NANOTCAD Project: Nanotechnology Computer Aided Design

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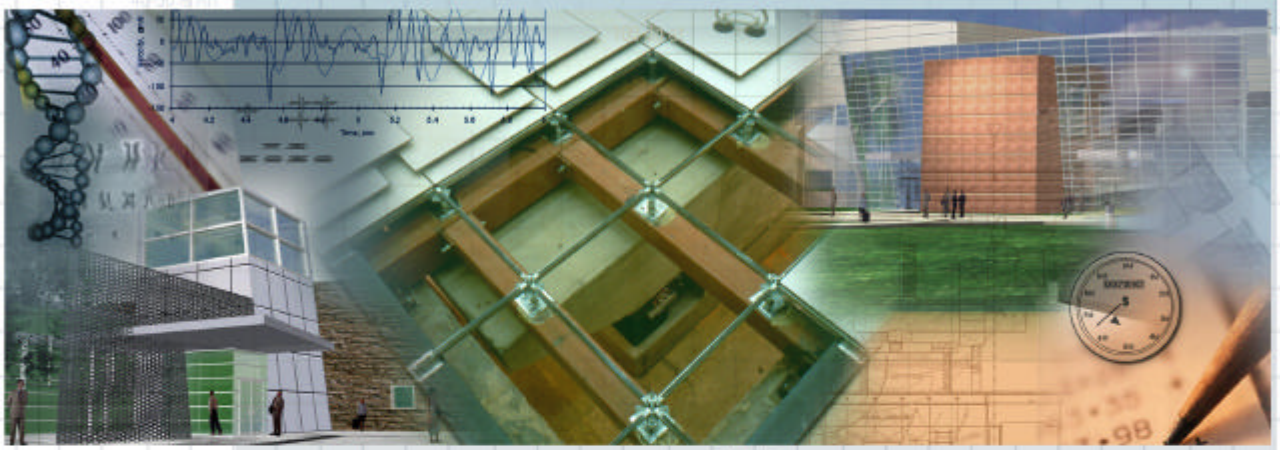

Arizona State University is hosting this year's **Buildings for Advanced Technology Workshop II** on January 21-23, 2004 following the great success of last year's BAT Workshop held at the National Institute of Standards and Technology (NIST) campus in Maryland, USA.

The conference will take place in the Mesa Centennial Conference Center, Mesa Arizona. The conference will focus on developing a connection between the emerging science and a range of technical factors to consider during the design and construction of advanced technology facilities supporting the next generation of **Nano-, Bio-, Micro- technology research and production**.

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INTRODUCTION

On behalf of the PHANTOMS team, I would like to wish all the network members Merry Christmas and Happy New Year 2004 hoping to see them at the 13th NID Nanoelectronics Information Devices (NID) workshop next year.

This event will take place in Athens (Greece) from the 4th to 6th of February 2004. Parallel and in collaboration with NCSR Demokritos, a joint Greek/Phantoms Nanoworkshop will be organised on Wednesday the 4th to present the latest advances in the Nanotechnology research areas addressed by the PHANTOMS network in this country.

The Organising Committee will also revitalise the Working Groups by having them contribute to selected roadmaps to be discussed at the workshop. We therefore encourage all the network members to actively participate to these new WGs ("Alternative Electronics", "Theory" and "Mono-Molecular Electronics") by sending contributions or submitting ideas.

The editorial board would like to acknowledge Giuseppe Iannaccone, Ricardo García and Anne Marie Bonnot as well as their collaborators for their contributions in this issue and to all the contributors who provided their input for this 14th issue of the PHANTOMS Newsletter.

This bi-monthly publication is supported by the EU-IST program within the PHANTOMS Network activities.

Antonio Correia (Editor)

PHANTOMS NEWSLETTER

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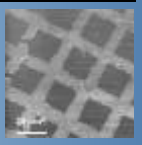

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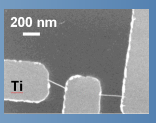

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NANOTCAD Project: Nanotechnology Computer Aided Design

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1. Introduction

The development of novel devices at the nanometer scale with potential for large-scale integration and room temperature operation is a formidable task. Over the years, many ideas have been proposed on the basis of very qualitative reasoning or simplified physical models: typically, the demonstration of working prototypes is achieved, while the fabrication of complex logic circuits proves to be unfeasible. While in some cases insufficient maturity of the available technology is responsible for the undesired outcome, most often fundamental problems are present. The extreme sensitivity of device operation to the presence of defects, stray charges, and other parasitics, the requirement of prohibitively tight fabrication tolerances, very slow switching times, or even the weakness of the physical effect on which the device is based, may easily prevent proper operation at large scale, or, possibly, at room temperature.

The NANOTCAD Project was mainly motivated by the prospect that many of the difficulties and of the limits of candidate technologies for nanoelectronics and molecular electronics could be predicted, anticipated and, hopefully, solved if detailed modeling tools of realistic devices and structures were available. The same modeling tools could be used to design more robust devices, and to select molecules and device structures with potential for use in large-scale integrated circuits. For these reason, the main objectives of the project were the following:

- Development and validation of a hierarchical set of software tools for the simulation and the design of a wide spectrum of devices, based on semiconductors and on transport through single molecules.
- Demonstration of a procedure for the realization of prototype nano-scale devices based on detailed modeling
- Design, fabrication, characterization and optimization of single and double quantum-dot HFET memories, resonant tunneling diodes, and nanoscale HFETs.
- Fabrication and characterization of devices in which transport occurs via one/few molecules connected to metal electrodes.

The project consortium consisted of six partners: four of them were directly involved in the theoretical activity of model and code development, and two partners were involved in the fabrication and characterization of state-of-the-art nanoscale devices and structures, to experiment a method for prototype realization and transport investigation strongly intertwined with nanostructure modeling. In detail, University of Pisa (DII-IET) and ETH Zürich focused on semiconductor modeling in quasi equilibrium conditions, for devices including subregions with different degree of quantum confinement (quantum dots, quantum wires, and quantum wells). ETHZ, in addition, focused on the coupling of quantum simulation based on density functional theory with commercial semiclassical TCAD tools of semiconductor devices, based on drift-diffusion and energy-balance transport models. TU Vienna was involved in the development of models and tools for Quantum Monte Carlo modeling, to account for far from equilibrium transport in quantum devices. NRMC Cork focused on molecular devices, developing a model and an associated numerical code for transport through single molecule that would not depend on a single particle picture or on a density function approach.

The experimental partners were the University of Würzburg, covering fabrication and characterization of semiconductors nanostructures and nanodevices, and Max-Planck Institut Stuttgart (MPG), covering the realization and characterization of devices in which transport occurs through single/few molecules. University of Pisa was in charge of Project coordination.

Project objectives have been largely met. A set of software tools have been developed and freely distributed to the european nanotechnology community through the Phantoms Simulation Hub (www.phantomshub.com) and comprehensive manuals have been prepared for non expert users. Such tools include codes for the self-consistent solution of Poisson-Schrödinger equation in semiconductor nanostructures with regions subjected to strong quantum confinement based on density functional theory (NANOTCAD1D, NANOTCAD2D, NANOTCAD3D), a quantum Monte Carlo code for the physically detailed simulation of one-dimensional devices operating in far from equilibrium conditions and in presence of strong dissipative phenomena (VMC), a code for the simulation of transport through single molecules contacted with metal electrodes immersed in a generic scalar potential (VICI), and a code for the three-dimensional simulation of semiconductor nanostructures (SIMNAD) coupled to a commercial drift-diffusion simulator (DESSIS$_{_ISE}$).

As far as semiconductor nanofabrication is concerned, significant results have been obtained: memories consisting of an AlGaAs-GaAs HFET with a single layer and a double layer of InGaAs quantum dots have been demonstrated,

with very fast write and erase times, and promising retention times. In addition, nanoscale FETs have been fabricated and characterized in which a unique signature of ballistic transport has been identified in the behavior of transconductance as a function of gate bias. A series of nanoscale devices have been fabricated that have allowed to validate and test the software tools developed within the project.
The molecular nanofabrication activity has successfully led to the demonstration of two techniques to fabricate a molecular device in which a small molecule bridges two metal electrodes separated by a gap of 1 nm. The first technique allowed contacting benzenedithiol molecules between two wires in a crossed geometry; the second technique allowed placing benzenedithiol molecules in nanogaps induced by controlled electromigration. In both cases it was possible to measure current-voltage characteristics exhibiting non-linear features close to those observed by other groups. Notwithstanding the intrinsically poor reproducibility of molecular structures, results achieved within NANOTCAD are at the state of the art in the field.

If nanotechnology will acquire industrial and economic relevance, it will strongly depend for its development on reliable Computer Aided Design tools, in the same way as Microelectronics relies upon TCAD tools. In that case, a broad basis of expertise in the development of CAD tools for nanotechnology - firmly established in Europe - would represent a real competitive advantage, with significant impact in terms of economic development and employment. NANOTCAD codes are tools for research and prototyping, but we believe their development has helped creating the necessary expertise on which a possible industrially oriented successor of the NANOTCAD project could be based.

2. Main Results of the project

Here we briefly review the main results of the project. The interested reader can find details in the final report, available on Phantoms website.

2.1. Development and release of NANOTCAD1D, NANOTCAD2D and NANOTCAD3D simulation programs for nanoscale semiconductor devices

Three programs have been developed for the simulation of semiconductor nanostructures in quasi-equilibrium conditions in one-, two-, and three-dimensional domains (NANOTCAD1D, NANOTCAD2D, NANOTCAD3D, respectively). All codes are based on the solution of the many-body Schrödinger equation with density functional theory, local density approximation, and allow subdividing the domain in several regions with different types of quantum confinement, providing a reasonable level of flexibility. In addition, NANOTCAD2D also allows the simulation of ballistic FETs both in the III-V and in the Si-SiO_2 material system [1].
During the project duration such codes have allowed to simulate several nanoelectronic devices fabricated within and outside the project, and to gain important insights into the transport mechanisms of such devices.

Particularly interesting results have been obtained in the simulation of quantum dot flash memories, both in the silicon-silicon oxide and in the AlGaAs-InGaAs material systems, of single electron transistors, of silicon-germanium quantum wires and of ballistic field effect transistors [2,3]. To provide some examples, Fig. 1 shows the typical structure of a silicon nanocrystal flash memories considered in a simulation and the relevant results as far as the stationary electrical properties of the device are concerned, i.e. chemical potentials and electron density in the channel as a function of the gate bias and of the number of electrons stored in the dots; Fig. 2 shows results from the simulation of a so-called "well tempered" MOSFET with channel length of 25 nm, used as a benchmark structure for comparison of different simulation methods.

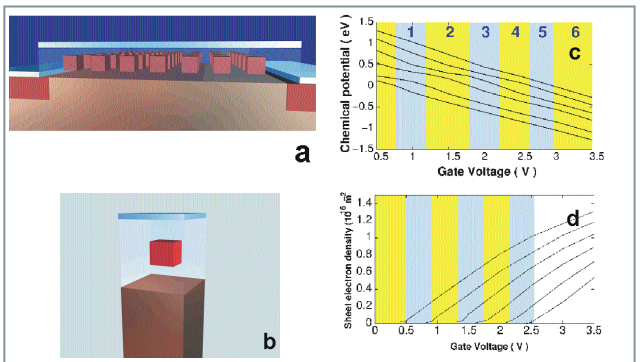

Figure 1: Simulation of silicon nanocrystal memories with NANOTCAD3D: a) simplified structure of a nanocrystal memories, in which disorder in nanocrystal size and density has been removed; b) elementary periodic cell considered in the 3D simulation; c) chemical potential of the dot as a function of the voltage applied to the top gate for number of electrons in the dot ranging from 1 to 6; d) two-dimensional electron density at the Si-SiO_2 interface as function of the gate voltage for an increasing number of electrons in the dot, from 0 to 5.

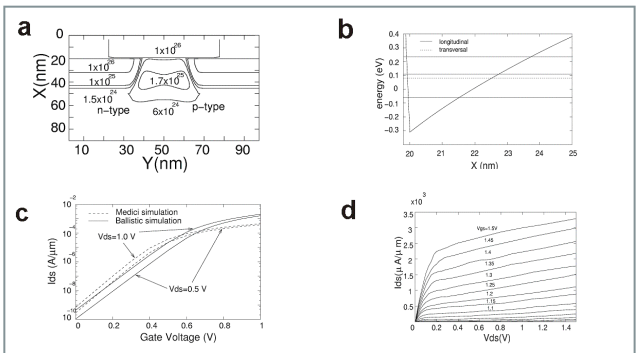

Figure 2: Results from the simulation of the 25 nm "well tempered" MOSFET: a) doping profile of the device; b) conduction band profile and energy levels of the two-dimensional subbands in the middle of the channel, from which the very strong quantum confinement is apparent; c) comparison between the transfer characteristics computed with the ballistic code and those obtained from simulations with the commercial simulator Medici; d) output characteristics of the device.

With respect to initial project objectives, several additional results have been obtained. Indeed, the simulation of nanoscale field effect transistors was not present among original objectives, but was included in the course of the project since after the first year it was very clear that the formalism and the tools developed for other ballistic devices such as quantum point contacts could be easily extended to include FETs [4]. In addition, a model for mesoscopic transport in the presence of decoherence, that was not an original objective of the project, was developed in order to achieve a better agreement with experiments as far as the

simulation of transport in coherent or quasi-coherent devices is concerned. On the other hand, the three-dimensional codes are not as fast as initially expected. This aspect actually limits the possibility of using them as a design tool, since it makes a detailed exploration of the design space unpractical.

Sinergy with other european and national projects has been very fruitful for access to experimental data, in particular with the EU Project ADAMANT, aimed at the development of silicon nanocrystal memories, and mainly focused on large scale fabrication and reliability aspects, and with the Italian Ministry of Research project "Single Electron Devices".

2.2. Development and release of a code for the simulation of transport through single molecules

A physical formalism has been constructed and implemented in the computer code package VICI which provides the capability to simulate two and three terminal molecular devices. The name VICI stands for *Voltage Current (I) in Configuration Interaction*. The two programs in the package are: analytic_integrals, a prerequisite integral generation code; and iv_Wigner_lm_penalty_function, the two- and three-terminal device simulator.

These codes are complex in internal operation but are based on a simple underlying physical formalism which minimises the number of adjustable parameters. What is most singular about these codes is that they operate genuinely at the *many-body* level: they do not rely on Density Functional Theory (DFT), an exchange-correlation functional, a Hartree potential or any Poisson-Schrodinger self-consistent cycle. They deal with N-electron many-body wavefunctions Ψ, and calculate matrix elements and expectation values of many-body operators exactly. The reason for the decision to attempt to implement a many-body formalism is that, since the beginning of the NANOTCAD project, the state-of-the-art in molecular transport calculations has evolved considerably from a simple tight-binding approach to an *ab initio* DFT-based method: the two most well-known methods are by M. Di Ventra et al. [5] and K. Stockbro et al.. [6] To produce a third usable code at this level would have been a significant achievement by itself, but the fact of the matter is that even with these state-of-the-art approaches, there are large (2-3 orders of magnitude) discrepancies between theoretical predictions and experimental measurements of IV characteristics of single molecules [5] and substantial disagreement even between these leading single-electron theoretical approaches. This motivated the decision to go substantially beyond all present formalisms and do a proper, first principles, treatment of the electronic motion of a current-carrying molecule. Even the very first runs of version 1 of the many-body code, in contrast, obtained the correct order of magnitude of the electric current flowing through the well-studied molecule benzene-1,4-dithiol.

The two programs developed within the NANOTCAD project require three preliminary calculations, two at the Density Functional Theory/Hartree Fock level (DFT/HF) and one at the Configuration Interaction (CI) level. An initial DFT/HF run is a standard requirement for all popular accurate many-body methods like CI or Quantum Monte Carlo (QMC), and there are many experienced research groups throughout the world who can perform such a calculation. Because the transport code is based on the CI formalism, the user would be well advised to spend some time learning the fundamentals of this approach to many-body theory. Once this is done, running the third preliminary calculation using the CI code mcci should not be too difficult.
Both the VICI codes are governed by user-friendly control files: in the case of analytic_integrals this can be simply one line in length. The transport code proper iv_Wigner_lm_penalty_function has a control file with more options, relating to the range of the applied bias, the gate field magnitude and direction, the number and position of the Wigner function constraints which capture the scattering boundary conditions, and some minimisation parameters for solving the central non-linear constrained optimisation problem. Compared to the typical number of parameters needed in running a DFT/HF calculation using a program suite like TURBOMOLE [7], this control file is very short, showing the simplicity of the underlying physical scheme.

Both the applied bias and the gate field are included exactly in the quantum mechanical many-body Hamiltonian, and the electric current is calculated exactly using the probability current density operator. What makes VICI code singular, as mentioned above, is that the exact matrix elements of the hard part of the Schrodinger equation-the electron-electron Coulomb repulsion- are included. Thus, it is possible, in principle, to find the *exact* solution of the Schrodinger equation for a molecular system: this is the main strength of CI, and therefore of the VICI package which is built on the CI formalism.

The code has been tested on a 38 atom gold cluster-benzenedithiol-gold cluster test system that has been well studied in the literature, of overall length 1.8 nm, obtaining on the very first runs currents of the same order of magnitude as experiment, and scaling up of the code in future versions is planned, so that larger systems can be studied. The main aim here is to simulate, atomically and with many-body accuracy, devices of the size of the commercial transistors of 10 years time, when the minimum feature size of the transistor should reach a few tens of nanometers or less. As already the exact Hamiltonian is included in the problem, there are no extensive changes to the code required in order to study Coulomb blockade, dopant fluctuations, or any other of the quantum effects that semiconductor companies are currently concerned about.

The ability to predict electronic transport on the nanoscale is relevant to IST projects concerned with the development of Ultimate CMOS technologies, whereby accurate quantum mechanical simulation is required for device design. Currently, theory and experiment for molecular electronic transport are difficult to reproduce. This statement applies to the repeatability of measurements, agreement between different theoretical treatments, and as well the agreement between theory and experiment. By producing a theoretical treatment that is parameter and approximation free, it will be possible to define repeatable and stable measurements

of currents for atomic scale devices. This will lead to the establishment of standards for the relationship of molecular and atomistic structure on electrical (current voltage) characteristics. Once these standards are established, and a firm understanding of device design on atomic scale dimensions is established, future technology generations extending beyond ultimate CMOS limits will be enabled.

2.3. Development and release of the SIMNAD code and coupling with standard semiconductor simulation codes (DESSIS$_{-ISE}$)

A common simulation environment for both drift-diffusion (DD) based devices (MOSFET) and single-electron tunneling devices would significantly enhance the modeling capabilities of standard TCAD tools in the nano range, which has up to now been out of scope for DD simulators. At the same time this would help in advancing new device principles as single-electron tunneling and in selecting the most promising designs for further applications.

With the substantial enhancements of the capabilities of the SET simulator SIMNAD [8] and the coupling to the commercial device simulator DESSIS$_{-ISE}$ this goal has been reached [9]. SIMNAD (SIMulator for NAnoDevices) is a quantum-mechanical 3D simulator for semiconductor devices based on a temperature-dependent effective mass formulation of density functional theory. It can be used to compute the self-consistent quantum mechanical charge density in semiconductor nanostructures, and can handle both direct gap materials (like III-V semiconductors) and materials with a silicon-like six-valley band structure and anisotropic effective mass. SIMNAD can calculate the full 3D wave function in MOSFET channels and SET leads based on the scattering matrix method with open boundary conditions. This can be used to compute the tunnel probabilities in SETs. Conductances computed by SIMNAD are either tunnelling conductances (e.g. in single-electron transistors) or quantum-ballistic conductances (e.g. in quantum point contacts or ballistic MOSFETs). SIMNAD uses a conductance model for Coulomb blockade devices based on the description by Beenakker (sequential tunneling) [10]. SIMNAD can also compute the coherent resonant tunneling current based on a modified Landauer-Büttiker formula. Currents through individual quantum point contacts can be obtained from a simplified ballistic tunneling model.

With a coupling-enabled version of the semi-classical device simulator DESSIS-$_{ISE}$ one can run simulations in coupled mode, i.e. SIMNAD will compute the quantum-mechanical charge densities for band profiles provided by DESSIS$_{-ISE}$ and will communicate this data back to DESSIS$_{-ISE}$ for further processing (e.g. for use in a DESSIS$_{-ISE}$ self-consistency iteration). This enables the simultaneous modeling of a (3D) quantum-mechanical charge distribution in a sub-region of a larger device, which is under full operation. Such a methodology is unique and no other comparable simulation package is known. In the non-self-consistent version of the coupling scheme, the quantum-mechanical charge density from SIMNAD is frozen-in for a subsequent DESSIS$_{-ISE}$ solve without any feedback. In the self-consistent version, the Poisson solver of SIMNAD is deactivated and the quantum-mechanical charge density is computed with the fixed potential obtained in a DESSIS$_{-ISE}$ run with the previous quantum-mechanical charge. The iteration is continued until convergence. The two simulators communicate via semaphor files, where DESSIS$_{-ISE}$ requests an update of the quantum-mechanical charge if required.

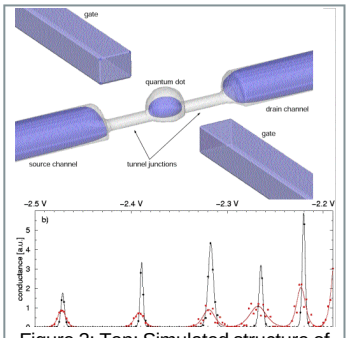

Figure 3: Top: Simulated structure of an SOI-SET. Blue indicates isocurves of electron density. Bottom: conductance versus gate voltage at 300 mK (black), and 1 K (red).

Semiconductor-based single-electron nanodevices both from III-V materials and from silicon represent a field of growing interest and a challenge in technology development. TCAD (Technology Computer Aided Design) is expected to become an increasingly valuable tool because of the immense difficulties (and costs) in producing nano-scaled devices with well-defined functionality.

The SIMNAD-DESSIS$_{-ISE}$ coupling might lead to a commercial software product in the future, provided that solid-state based nano-electronics will reach an industrial level. On the other hand, the necessity to model quantum effects on a sound physical basis is also given by the foreseen development in CMOS technology: SOI devices with ultra-thin silicon layers and ultra-short channels, which exhibit a truly three-dimensional distribution of charge density, potential, and current density, will become dominant soon. Users of TCAD tools will demand for 'first-principle' quantum transport models, since they will mistrust the above-mentioned approximate methods available today.

2.4. Development and release of VMC: a code for Monte Carlo simulation of quantum transport

A novel MC method for the solution of the Wigner-Boltzmann equation [11] has been integrated in the one-dimensional device simulator VMC (Vienna Monte Carlo code). The concepts and features of the simulator, input deck and out files are described in a user's guide. The basic input quantity is the profile of the conduction band edge in the device. This profile can either be specified analytically in the input deck, or, for the purpose of a self-consistent simulation, be read from an input file, which is typically generated by a Schrödinger-Poisson solver. The simulator VMC is released by the Institute for Microelectronics (www.iue.tuwien.ac.at). The simulator can also be accessed on the Phantoms simulation hub.

The Wigner-Boltzmann equation for electrons in semiconductor devices is solved numerically by means of a novel Monte Carlo method. This equation describes both quantum interference and dissipation effects due to carrier scattering. The methodology for deriving the method is summarized in the following. The integral form of the Wigner-Boltzmann equation is used as a starting point for. The kernel of the adjoint equation has been decomposed into a linear combination of conditional probability densities. These densities represent the transition density used for the construction of numerical trajectories. The properties of the transition den-

sity employed allow a particle picture to be introduced. In this picture dissipation and interference phenomena are taken into account by two alternative processes involving quasi-particles. Dissipation caused by interaction with phonons and other scattering sources is accounted for by drift and scattering processes corresponding to the semi-classical Boltzmann transport picture. Interference effects due to the Wigner potential are associated with generation of pairs of particles having statistical weight ±1. The classical force term is separated from the Wigner potential and included in the Liouville operator.

With this modification, the developed model corresponds to a Boltzmann equation augmented by a generation term. The challenge of employing such method is to handle the avalanche of numerical particles properly. The problem has been solved for stationary conditions: Particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation. The cancellation is due to the fact that such particles have a common probabilistic future but opposite contribution to the statistics.

The novel MC method has been validated by comparison with NEMO-1D, a well-known simulator based on the non-equilibrium Green's function technique and developed in the US [12]. Different types of resonant tunneling diodes have been used as benchmark devices. In some cases phonons scattering is found to play an important role, as predicted by both simulators. Simulation results are also compared with measurements of a RTD fabricated and characterized within this project by the team in Würzburg. Reasonable agreement is found for the resonance voltage and peak current density. Software developed in the US and funded by national US agencies is often not available outside the US. The tools developed in NANOTCAD are therefore a valuable design aid to be used by European industry and research institutions.

2.5. Fabrication and characterization of Flash Memories with a single and a double layer of quantum dots

Within the first period of the project single quantum dot flash memories (QDFM) were realized by molecular beam epitaxy of modulation doped GaAs/AlGaAs heterostructures with self assembled InGaAs quantum dots embedded in the spacer. Nanoscaled devices controlled by in situ defined side gates were realized by electron beam lithography and etching techniques with 70 nm wide channels controlled. It is found that the drain current threshold differs by up to 2 V with respect to down and up sweeps of the gate voltage. The large hysteresis is attributed to charging and discharging of the quantum dots in the spacer and persists up to 260 K [13].

Most of the publications related to QD memory devices have studied concepts involving several hundreds of quantum dots implemented in an self-assembled manner, e.g. as Si-nanocrystals [14-16]. So far, only a very limited number of publications reported on memories with feature sizes of only a few self assembled quantum dots [13,17].

The layout of the structure was optimised by NANOTCAD simulation tools. As a result a 2QDFM was designed (shown in Fig. 4) which shows wide memory window (Fig. 5). The NANOTCAD simulation tools were proofed to describe nanoscale devices and supported the improvement of the layout with respect to a better functionality of the QDFM.

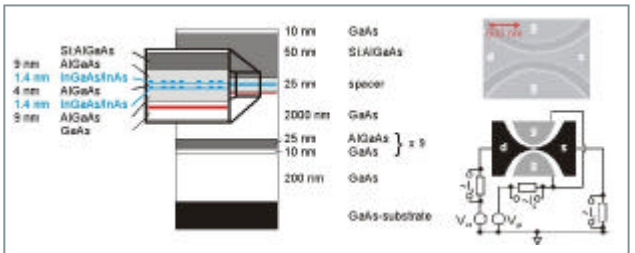

Figure 4: Left part: Schematic cross-section of a GaAs/AlGaAs modulation doped heterostructure. Within the spacer 2 InGaAs self-assembled quantum dots (QD) layers have been embedded. The 2QD layers are 4 nm apart with the first layer separated 9 nm from the GaAs/AlGaAs interface with beneath residing a two dimensional electron gas (2DEG). Right part: An electron micrograph shows a top view of an etched constriction. Two lateral side gates are separated from the channel by trenches. The electrical setup is sketched in the lower part.

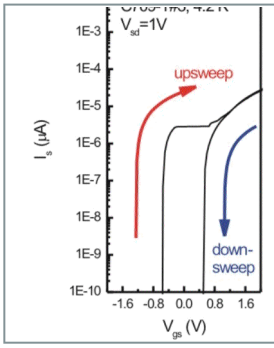

Figure 5: The current versus voltage (I-V) characteristics for up and down sweeps of the gate voltage. The gate voltage, V_{gs}, was varied between -3 V and +5 V. The onset of the source current, I_S, depends sensitively on the sweep direction of the gate voltage. The resulting hysteresis of the I-V-trace is V_{hys} = 1.07 V.

2.6: Fabrication of two-terminal molecular devices and assessment of techniques for contacting single molecules

Within the molecular nanofabrication activity, the main research goal was the measurement of electrical transport through a small molecule (benzene-ring with two functional groups) bridging a metal electrode gap whose length is below 1 nm. Such tiny electrode separation is far beyond the lithographic resolution available today.

To approach this task, the following two contact configurations were realized:

- Benzenedithiol molecules were incorporated between two nanowires arranged in crossed-geometry (sandwich junction). Here the formation of short-circuits was successfully avoided trough an appropriate method for assembling the molecules onto the bottom contact.
- Contacting of benzenedithiol molecules inside nano-gaps created within nanowires of small, well-defined dimensions. The electrical resistance observed after electromigration-induced breaking of nanowires coated with a molecular film was smaller than in the absence of the molecules, indicating the successful incorporation of the molecule(s).

In both contacting methods, gold/palladium (AuPd) nanowires (8 nm in height, ~ 15 nm in width) were used as basic constituents. These wires were fabricated by a newly developed template-based method, which employs transi-

tion metal oxide nanowires as removable etching masks to pattern the underlying AuPd layer, as schematically illustrated in Figure 6 [18]. This approach allows for the fabrication of homogeneous wires with clean surface, which cannot be directly achieved by e-beam lithography techniques.

For both contact configurations the I/V characteristics exhibited features such as kinks or steps at low temperature (2 K). In addition, most of the I/V curves showed a well-developed gap around zero bias. Figure 7 depicts two representative I/V traces, belonging to a crossed-wire and nano-gap junction, respectively. The following observations support the conclusion that these features could be a signature of transport through molecular states:

- the differential conductance curves (dI/dV) resemble those reported by other groups [19] in that the first peaks for positive/negative bias are almost symmetric around zero bias;
- peak differential conductivity values in the µS range have been obtained (almost independent of temperature), which is the same order of magnitude as reported by others [20-22].

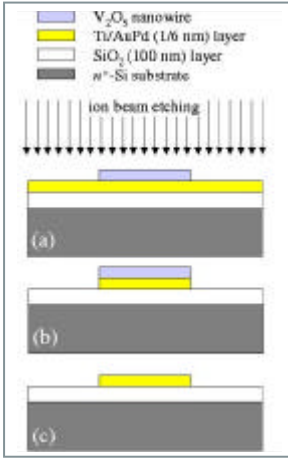

Figure 6: Schematic illustration of the nanowire fabrication process. (a) Vanadiumpentoxide (V_2O_5) nanofibers are employed as an etching mask on top of the thin AuPd layer. (b) AuPd film regions unprotected by the etching mask are removed by argon ion beam etching. (c) Remaining parts of the V_2O_5 wires are removed with a dilute acid solution.

However, care has to be taken when interpreting these results, since a low reproducibility was observed between different junctions comprising the same molecule(s), i.e. a different number of features occurred at varying voltage positions in the I/V traces. It is believed that the low reproducibility constitutes a general, intrinsic problem. The apparent consistency between the results reported by other groups may be due to a selection from a pool of diverging data (it is noted that only in rare cases the low reproducibility has explicitly been admitted [23]). Furthermore, the molecule-electrode interface appears to play a dominant role [24].

In addition to aforementioned complications, no gate effect on conductance could be observed (for 100 nm back gate separation), which would be required for three-terminal devices. This observation is ascribed to the strong electrostatic shielding associated with the closely spaced contacts [23].

Nonetheless the work performed within NANOTCAD is expected to allow for further basic research possibilities, and perhaps even to catalyze some technological applications. For instance, the electrodeposition method devised for coating metallic nanowires with molecular films of controlled thickness should be applicable to various types of mono- and bifunctional molecules, and therefore may stimulate the fabrication of devices with mid-term prospect for industrial application. One example could be the further development of memory arrays based upon crossbar structures, requiring molecules that are usually hard to assemble by conventional methods (spin coating, Langmuir-Blodgett films).

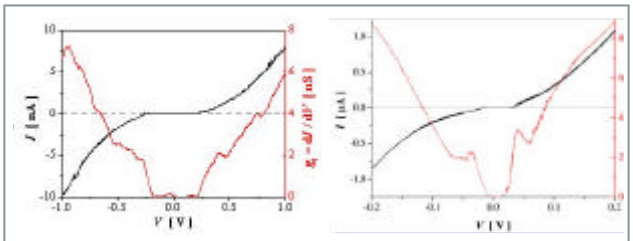

Figure 7: Low temperature current-voltage (I-V) and differential conductance (g_d) curves of a molecular junction made by electrochemical deposition. The bottom electrode has been electrochemically coated with 1,3-benzenedithiol molecules from an ethanol solution. The sample was cooled down to T = 2.0 K in order to suppress the noise. Right: Two-probe low temperature (T = 2.0 K) transport properties of a single-molecular junction fabricated by breaking an AuPd nanowire (15nm width) via electromigration. The 1,3-benzenedithiol molecules have been deposited on the nanowire by an electrochemical procedure prior to breaking. In both cases, the differential conductance was measured by a lock-in technique.

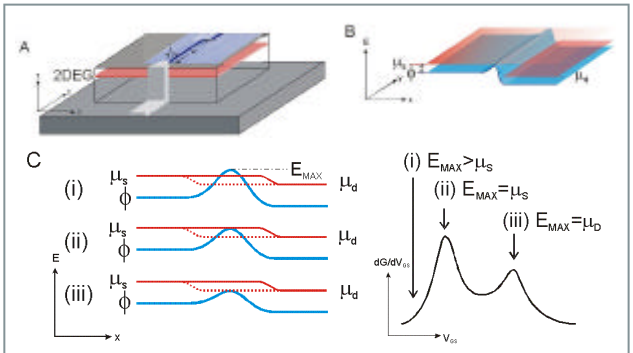

Figure 8: Schematic representation of the field effect transistors with scanning electron micrograph showing the gate section, at which the tapered gate is discharged into the narrow, top gate.
A: Gate structures with lengths down to 20 nm and widths of 100 µm guarantee that gating effects from outer device regions are not important. A two-dimensional electrons (2DEG) 120 nm below the sample surface is controlled by the gate. Electrons can pass the channel between the source and the drain without suffering losses in their energy and momentum.
B: The conduction band pattern Φ of the 2DEG is shifted by the voltage difference between the drain and the source $V_{DS} = (m_S - m_D)/e$ with m_S and m_D the chemical potential of electrons in the source and the drain, respectively.
C: Sketch of subband profiles for interpretation of the experimental results: (i) Profile of the lowest two-dimensional subband in the HFET channel for low gate voltage. Since the subband maximum E_{MAX} is larger than both m_S and m_D the device is in cut-off. (ii) As VGS is increased, the subband maximum E_{MAX} decreases. When E_{MAX} goes below m_S the conductance increases abruptly. Therefore the first peak of dG/dV_{DS} occurs. (iii) As V_{GS} is further increased, E_{MAX} goes below m_D and the conductance increases faster, since now the electron flux is limited only by the availability of empty states at the drain, and not by the channel barrier. For further increases of V_{GS} the conductance saturates to the contact resistance.

2.7. Characterization and demonstration of a universal signature of ballistic transport in nanoscale field effect transistors

Field effect transistors (FET) with gate lengths down to 20 nm have been fabricated and FET operation in the ballistic transport regime has been demonstrated. An unforeseen transport feature has been observed on the basis of four-terminal measurements that allows one to identify that the device at hand is a ballistic FET (Figures 8 and 9). Using the presented NANOTCAD programs it was possible to model this ballistic effect for the first time demonstrating the precise description of the relevant physics. Due to the underlying ballistic mechanism, it has been shown that FETs do work in the ballistic regime [25].

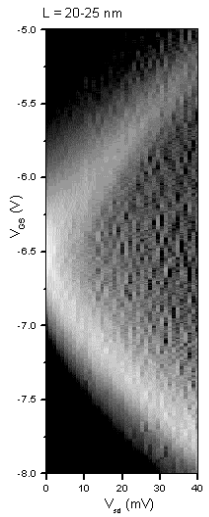

Figure 9: Specific peak splitting of the derivative of the differential conductance for constant drain to source bias voltage V_{DS} of ballistic field effect transistors. Grey scale plot of the derivative of the differential conductance for FET with 25 nm gate length. The splitting is clearly seen and increases linearly with the applied source to drain voltage V_{DS}.

3. Conclusion

The NANOTCAD package has been developed as a hierarchical set of tools. All tools have been prepared and freely delivered to the nanoelectronics community through the PHANTOMS Simulation Hub (www.phantomshub.com) or, in the case of one code using proprietary routines (SIMNAD), are freely available to those institutions with a licence of ISE-TCAD. Comprehensive manuals have been prepared for all tools and available for download on the project site (nanotcad.iet.unipi.it) and on the PHANTOMS hub. In addition, a tutorial session on tools developed within NANOTCAD has been organized during the NID Workshop in Cork, and a presentation with a tutorial part on NANOTCAD tools has been given at the International School MIGAS “Towards Nanoelectronics" held in Autrans 14-20 June 2003.

Let us finally highlight the fact that, beyond the development of simulation tools, the theoretical investigation of transport in nanostructures and the fabrication of semiconductor and molecular nanostructures have produced results that have significantly advanced the state of the art.

Acknowlegments

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Bridging nano and macro worlds with water meniscii

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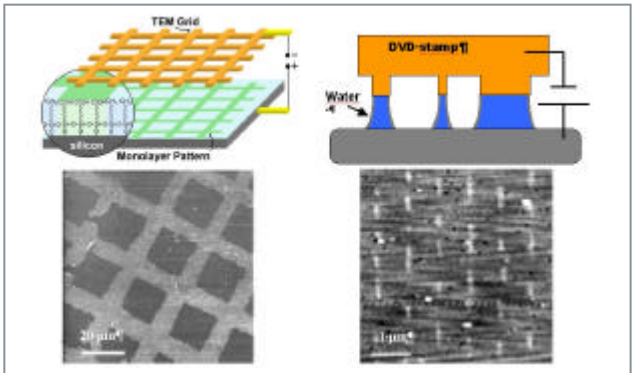
What once was a nuisance in surface and material science, the spontaneous absorption of water on surfaces, is now a key element of a powerful method to fabricate sophisticated quantum devices with a large-scale patterning potential.

From the sophisticated monitoring of attractive van der Waals forces to the control of atomic positions, and from the crude approach of scratching surfaces by ploughing a nanometer-sized tip, the scanning probes have generated a fascinating variety of methods for atomic and nanometer-scale manipulation and modification of surfaces [1]. However, technical requirements such as the use of vacuum and low temperatures have rendered many of these methods of little practical relevance. Furthermore, the sequential character of scanning probe operation and the limited area covered by a single tip (~10^4 μm^2) restricts its usefulness for patterning large scale areas. It is rather natural to attempt the scaling of the techniques with large arrays of cantilevers [2]. This is a viable approach, however parallel operation of large cantilever arrays is complex. Hoeppener and collaborators [3] at the Weizmann Institute (Israel) and Cavallini and colleagues [4] from a joint CNR (Italy)-CSIC (Spain) collaboration have used a different approach. Rather than arrays, they propose to scale the physical process and print simultaneously multiple sites. Both teams have chosen the same physical process, the site selective oxidation of a surface. This process is the basis of a robust and versatile probe-based method for modifying surfaces, generally known as Local Oxidation Nanolithography.

Local oxidation is based on the spatial confinement of a chemical reaction (oxidation) within the walls of a water meniscus formed between an atomic force microscope tip-sample interface. The formation of the liquid meniscus may be driven by thermodynamic considerations in the presence of tip-sample mechanical contact or by the application of an electrical field when tip and surface are several nanometers away [5]. The method to form liquid bridges is so precise that meniscus diameters of 20 nm are easily obtained. This has lead to the reproducible fabrication of 10 nm structures [6]. Since its inauspicious discovery [7] in the heydays of atomic-scale manipulation of surface by scanning tunneling microscopy, the method has evolved to challenge electron beam lithography in the fabrication of devices for studying a variety of quantum phenomena such as coulomb blockade, quantum conductance and alike [8].

Weizmann and CNR-CSIC teams have replaced the single asperity geometry of an atomic force microscope for a multiple protrusion system (a stamp) and then pressed the stamp against the surface to transfer the features on the stamp. The Weizmann group used a TEM copper grid with 10 µm bars for the stamp. The patterned surface was a highly ordered organosilane monolayer self-assembled on silicon. The application of the appropriate voltage converted the selected site from methyl terminated groups on the monolayer underneath the copper bars to carboxyl groups, thereby replicating the stamp features. The CNR-CSIC team went a step further by using a stamp with submicrometer features, actually a piece of a digital video disk (DVD). By exerting a pressure of several kg/cm^2 between the stamp and a silicon surface while applying an external voltage, they were able to transfer all the bits of the DVD on a silicon surface over a 5x6 mm^2 in a process that lasted about 15 s. In the Italian-Spanish approach the transferred motives were about twice as small as the original protrusions of the stamp and this led to the patterning of 100 nm features. In both cases it was surprising to learn that there was enough water absorbed on the surfaces to form millions of water meniscii.

Parallel local oxidation is conceptually simple, low cost and can be applied to modify a large variety of metallic, semiconducting and organic self-assembled monolayers surfaces. It benefits from the established knowledge of imprinting lithography's and scanning probe-base oxidation so it seems reasonable to expect future applications in technology. But implications aside, it is remarkable to learn that field-induced formation and manipulation of tiny water bridges can be used to fabricate the mesoscopic and nanometer-scale devices to study quantum phenomena.



Schematics and results of two parallel local oxidation processes. The monolayer imprint on the left is the result of converting surface exposed -CH_3 to -COOH. The right image shows the transfer of DVD bits to a silicon surface by the local oxidation of the surface under the DVD protrusions.

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Self assembled single wall carbon nanotube Field effect transistors and AFM tips prepared by Hot Filament assisted CVD

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We have developed a Hot Filament CVD (HFCVD) technique to grow single wall carbon nanotubes (SWNT) in the presence of a thin catalyst layer [1, 2]. As an example of the performance of the technique, fig. 1 shows an isolated SWNT suspended between Si pillars and the corresponding Raman spectrum for a 1.96 eV He-Ne laser radiation.

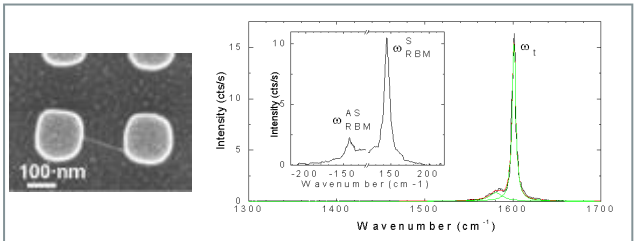

Fig. 1 : SEM image (left) and Raman spectrum(right) of isolated suspended SWNT. The RBM Raman peaks at ω_{RBM} ± 145 cm^{-1} indicate a d=1.7 nm SWNT (d (nm)=248/ω_{RBM}(cm^{-1})).

The absence of any Raman signal of defective carbon around 1300 cm^{-1}, with the narrowness of the tangential line at ω_t = 1601 cm^{-1} (5 cm^{-1} width at half maximum) are the indication of the high purity and crystallization of the SWNTs.

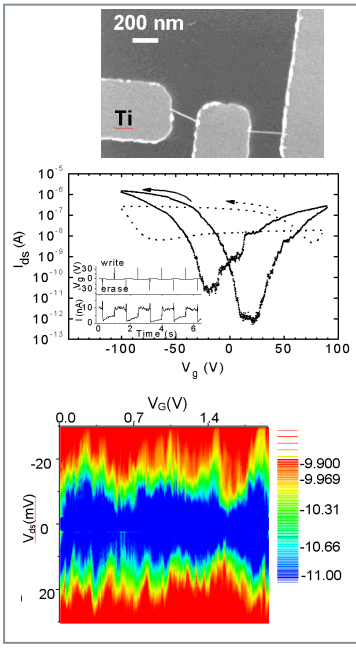

Fig. 2: Top : FE-SEM image of a typical sample. Middle: Backgate dependence of the drain-source current at T=300K V_{ds}=50mV (dotted line) and T=1K and V_{ds}=+1V (solid line). Arrows indicate the hysteresis direction. Inset: writing-erasing of a "bit" in a "CNFET memory" at 300 K by applying gate voltage pulses of 34 V and 10 ms long at 300 K for a drain-source bias voltage of +40 mV. Bottom : Map of the drain-source current at 4K with respect to the low drain-source bias (vertical axis) and of the backgate bias (horizontal axis). "Coulomb Diamonds" are signature of single electron effects.

NTFETs (fig. 2) were fabricated in a two steps process: a first one for designing Ti electrodes with a thin top layer of metallic catalyst using e-beam lithography, a second one for in situ wiring a suspended nanotube to the Ti electrodes using the HFCVD growth technique. Electronic transport properties were then measured directly after the growth, without any post treatment.

NT tips (fig. 3) were prepared by HFCVD growth on commercial Si tips using similar HFCVD condition. The peculiarity of the technique is to lead to the growth of a unique SWNT bundle at the apex of the Si tips.

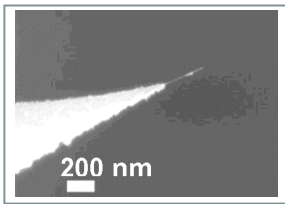

Fig. 3 : SEM image of a SWNT grown at the apex of an Si tip

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TNT2003 Selected Abstracts

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COLD CATHODES, THE NEW APPROACHES FOR NANOTECHNOLOGY

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Electron sources of high current density and high efficiency are the main element of numerous applications in power vacuum tubes, electron microscopes and information displays. Based on the working temperature, electron sources can be classified into two main groups. The first one is the hot cathodes in which the material is heated to such a high temperature (>1000 K) that a small fraction of electrons has sufficient energy to overcome the work function of a metallic cathode [1]. The second one is the cold cathodes which emit electrons at room temperature (RT), or lower, and include a large variety of types based either on field emission tunneling mechanism, on p-n junctions, on photo-excitation, on negative electron affinity of the surface and on secondary emission, to cite only some of them [2].

Since the concept of vacuum microelectronics, proposed in 1961 by Shoulder [3], and the introduction of "Spindt cathodes" [4] that have shown the feasibility for the fabrication of large area cold cathodes, a regain in the interest for vacuum microelectronics was observed from the 1980's. The main reason is the possibility for extreme miniaturization of cold cathodes that could lead to numerous technological breakthroughs. Among them, some applications have generated recently a huge effort in research and industrial developments: such as flat panel field emission displays (FED's), high power vacuum tube amplifiers, microguns and inverse Nottingham cooling devices, to mention only the principal.

However, industrial development of vacuum microelectronics devices is more demanding than the academic uses of field emission (FE) for surface studies, by FE microscopy for example. Considering the different applications that used electron beams, an ideal cathode, from the industrial point of view, can be outlined with, in particular, the possibility of high throughput and ease of fabrication for large area cathodes, a condition needed for the commercial success of any emitter.

To meet these requirements, novel electron cold sources have been proposed. In this presentation we restrict the discussion to FE cathodes using individual carbon nanotubes (MWNT) and to planar cold cathodes, the recent solid-state field-controlled emitters (SSE), for which the emission barrier is mainly controlled by the solid state electronic properties of the layer just underneath the surface.

Individual multi-walled carbon nanotubes were obtained when the size of the catalytic metal clusters was in the order of the diameter of the MWNT's, i.e. less than 100 nm. Their growth direction was preset by the direction of an electric field applied during the process [5]. This technology was developed within the context of an European project, Nanolith [6], and has shown an uniformity and a yield of nearly 100 % for the fabrication of a 2-D array of these individual MWNTs. Each of these CNTs, due to their aspect ratio, was a good field emitter that, after a seasoning process, mostly ended to the same field emission characteristics equivalent to a metal-like tip having a work function $\phi \cong 4$ eV [7].

Field electron emission requiring low electric field represents a big challenge for applications running from the realization of field emission planar structures through local cooling by using inverse Nottingham effect [8, 9, 10] without surface structuring such as ultra-sharp tips or ridges. The conventional approach was to modify the metal surface barrier by the surface adsorption of polarized species such as alkali metals for example [11]. Our alternative new approach, called solid-state field-controlled emission (SSE), is to modify the electronic properties of the underneath surface layer in order to control the surface emission barrier and gave stable emission characteristics with low threshold fields. These SSE cold cathodes consist either of a single ultra-thin layer of a large gap semiconductor [12], or nanostructured composite layers recently developed with the group of Tsu of the University of North Carolina at Charlotte [13]. The experimental results were interpreted within new schemes of electron emission mechanism.

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COHERENT EMISSION OF THERMAL LIGHT BY MICROSTRUCTURES

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It is usually taken for granted that light spontaneously emitted by a thermal source such as a light bulb is spatially incoherent. In other words, it is generally assumed that fields produced by different points of a thermal source cannot interfere. By contrast, different points of a radio antenna emit waves that interfere constructively in particular directions producing well-defined angular lobes. The intensity emitted by a thermal source is the sum of the intensities emitted by different points so that it cannot be directional. Since the currents generating the thermally emitted fields are due to uncorrelated random thermal motion, it seems that a thermal source cannot be spatially coherent or directional. However, it has been shown recently by Carminati et al. (1999)[1] and Shchegrov et al. (2000)[2] that the field generated by a plane interface at temperature T may have a large coherence length and can be quasi monochromatic in the near field. This paves the way for the construction of a thermal source that could radiate light within narrow angular lobes as an antenna instead of having the usual quasi lambertian angular behaviour. In this paper, we will report experimental measurements demonstrating that it is indeed possible to build an infrared antenna by ruling a grating on a polar material such as a semiconductor. Such an antenna radiates infrared light in a narrow solid angle when it is heated as shown in Figure 1. This is a signature of the spatial coherence of the source. We will discuss the physical origin of the spatial coherence of the thermal source. We will in particular show that this effect is due to the excitation of a surface wave.

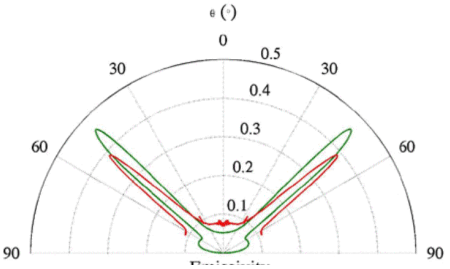

Figure 1: A grating with period 0.55 λ and height λ/40 where λ=11.36 µm has been ruled on a SiC interface.The figure represents the emission at 11.36 µm in p-polarization as a function of the emission angle. The source temperature is 773 K. The intensity is normalized by the intensity of a blackbody at same temperature. The curves show the theory (green) and the measurements (red). The discrepancy is due to the use of the index at ambient temperature in the theory. It is seen that the angular pattern displays narrow lobes like an antenna.
This is a signature of the spatial coherence of the source. Reproduced from ref.[3]

Another remarkable property of this source is that the emissivity is enhanced by a factor of 20 compared to the emissivity of a flat surface. No enhancement is observed for s-polarized light. Finally, we will show that the emission spectrum depends on the observation direction. We will also discuss the possibility of designing quasi isotropic source with very high emissivity.

All the above properties are fundamentally related to the surface-phonon polariton and can be summarized by its dispersion relation. We will report measurements of the reflectivity spectra as shown in Figure 2 that allowed us to measure the dispersion relation. Using this dispersion relation, we will discuss possible applications to the design of efficient photovoltaic cells, infrared sources in the far field and in the near field and enhanced radiative heat transfer at short distances.

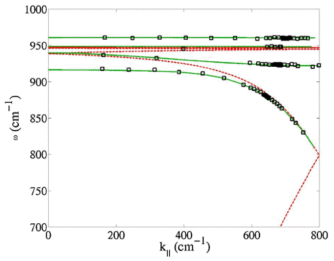

Figure 2: Dispersion relation of the surface phonon polariton on the grating. Markers: experimental points. Dashed red line: theory for a plane surface; Plain green line: theory for a grating. Note the presence of a gap in the case of a grating. As a consequence, the higher branch is almost flat. Reproduced from ref.[3]

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ELECTRONIC STATES AND THEIR CONTROL IN SEMICONDUCTOR QUANTUM DOTS

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Quantum nanostructures, such as quantum dots, have become key structures for future semiconductor devices and quantum information technology. Transport characteristics of quantum dots have been extensively studied by conventional conductance measurement as a function of gate bias and magnetic field. Many interesting physics, including the atom-like behavior of quantum dots [1], have been revealed in the last decade. Recently, these studies have been extended to include direct monitoring and pulse control of electronic states in semiconductor quantum dots. These techniques are essential to understand nanoscale features, to study carrier dynamics, and to realize coherent control of electronic states in quantum dots.

Direct nanoprobing of electronic states is not possible in conventional quantum dots, which are buried inside of semiconductors. However, electron gas accumulates just beneath the surface for some semiconductors like InAs (111)A [2]. A tetrahedral defect in InAs (111)A film operates as a triangular quantum dot and the local density of states (LDOS) of each zero-dimensional state can be visualized by using low-temperature STM [3], as shown in Fig. 1. Nanoscale properties of the quantum dot become clear through these observations. Recently, we measured the coupling characteristics of electron waves using a laterally coupled double-dot system.

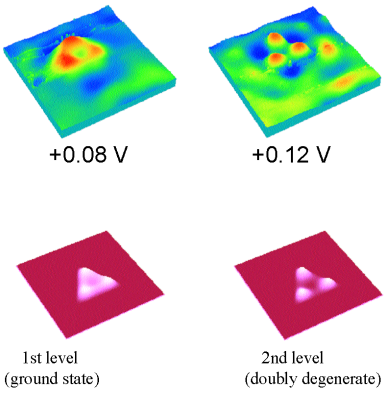

Fig. 1 LDOS distribution of the first and the second zero-dimensional states observed in the quantum dot with a side length of 17 nm. Theorical simulation (bottom) agrees well with experiments.

The detailed electronic states, i.e., orbital and spin states, have also been identified for a circular quantum dot called artificial atom. We developed an electrical pump-and-probe technique for quantum dots and measured the electron dynamics of artificial atoms. In an artificial hydrogen, the measured electron relaxation time from the excited to the ground state was is around 10 nsec, reflecting phonon assisted relaxation. The electron spin is conserved during the relaxation in this case. On the other hand, the relaxation of an artificial helium includes a spin-flip process and the measured relaxation time is around 200 µsec. Such extremely long relaxation time indicates that spin-flip relaxation is strongly forbidden in semiconductor artificial atoms like real atoms [4]. The large difference in relaxation time between spin-conserved and spin-flipped relaxations has also been widely observed in conventional quantum dot systems [5], suggesting that electron spin is well isolated from the circumstances.

We also applied the electrical pump-and-probe technique to measure the coherent oscillation of an electron in a coupled-quantum-dot system, where electron occupation in right or left dot operates as a quantum two-level system. The first pulse, i.e. the initialization stage, puts the electron in the left dot. Then, the system is set to the resonant condition during the second pulse. We successfully observed a current oscillation depending on whether electron locates in the left or right dot as a function of the duration of the second pulse [6], as shown in Fig. 2. Furthermore, we demonstrated modulation of the oscillation frequency and arbitrary control of the pseudospin rotation on the Bloch sphere by changing the electrical signal applied to the system [7]. This is the first demonstration of an electrically controlled semiconductor charge qubit.

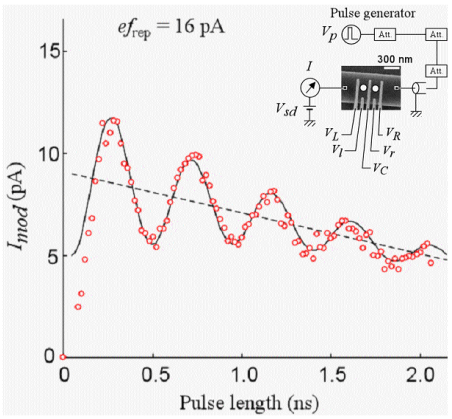

Fig. 1 Coherent oscillation of an electron observed in a coupled quantum dot system. The inset is a schematic diagram of the experimental setup.

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FOCUSED ION BEAMS : APPLICATIONS IN NANOTECHNOLOGY

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Worldwide efforts in Nanotechnology are gaining further momentum as new instruments in nanofabrication are introduced. Focused ion beam (FIB) microscope is widely used for patterning various nanostructures because it offers a greater flexibility than traditional methods by allowing dry and maskless etching on a nanometer scale with a surgical precision. We have explored the FIB technology to realize novel applications in nanoelectronics [1,2] (See for example, Fig. 1), photonic devices [3-5] (Fig. 2) and bionanotechnology (Fig. 3). We will go over a wide range of projects being carried out in our centre from lower level modification to key device enabler. We will address its limitations and potentials in the future development of nanotechnology.

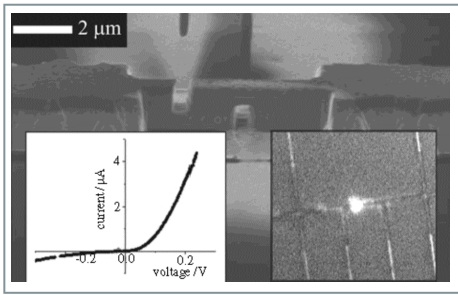


Fig. 1: FIB image of nanoscale GaN LED. Inset: the I-V characteristics of the device and an optical image of the glowing LED with bias current.

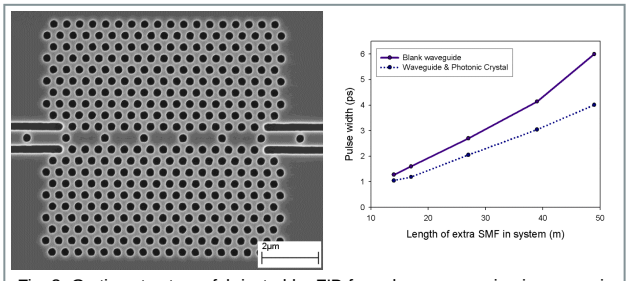
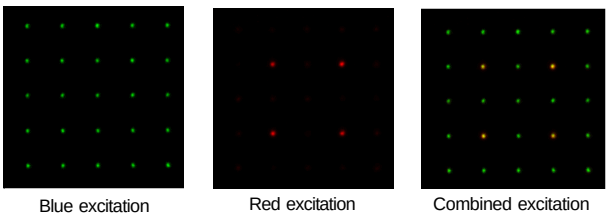


Fig. 2. Grating structures fabricated by FIB for pulse compression in waveguide devices



Blue excitation | Red excitation | Combined excitation

Fig. 3. Fluorescent microscope image of FIB holes in Au (50 nm) ; holes are filled with thiols + IgG + anti-IgG using nano-pipette (10 nM), (line scan, about 1 min- 500 mV in 30 x 30 µm^2)

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MATERIALS ISSUES IN NANOLITHOGRAPHY

Phantoms

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The trends towards ultimate miniaturization in semiconductor technology and the fabrication challenges in nanotechnology call for new approaches and materials which enable the fabrication of nanometer sized structures. One of the most widely used technologies to generate such patterns is electron beam lithography where an electron beam with a potentially sub-nanometer diameter is scanned over the substrate coated with a polymeric resist layer. The smallest obtainable structure size not only depends on the beam diameter but also on the resist resolution, determined to a large extent by its building blocks. Therefore research and development in the field of nonpolymeric high resolution electron beam resists is of high interest. In a series of publications [1 - 3] it has been shown that calixarene derivatives used as negative tone electron beam resists have the potential to pattern down to the 10 nm regime an below (e.g. see fig. 1).

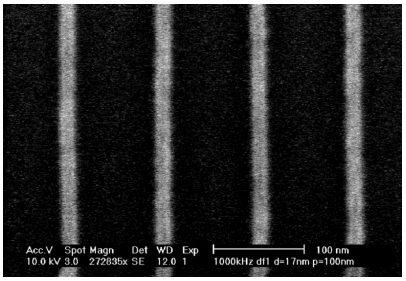

Figure 1: 17 nm lines fabricated from tetra(bromoacetoxy)calix[4]arene

Our current research is focused on ways to reduce the required electron dose which is almost three orders of magnitude higher for calixarene derivatives compared to commercial polymeric resist materials [2,3]. Systematic studies on the effect of various chemical modifications on practical parameters such as sensitivity and etching resistance have been performed. A significant has been obtained from adapting the commonly used technique of chemical amplification [4] based on catalyzed kationic polymerisation of epoxy derivatives to this class of materials, resulting in a sensitivity enhancement by two orders of magnitude for tetraepoxy-tert.-butylcalix[4]arene (fig. 2). At this point this chemically

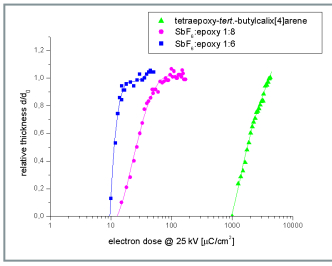

Figure 2: Remainig relative resist thickness vs. dose for different PAG concentrations

amplified resist still has high resolution capabilities by yielding 40nm lines and spaces without any further optimization (fig. 3).

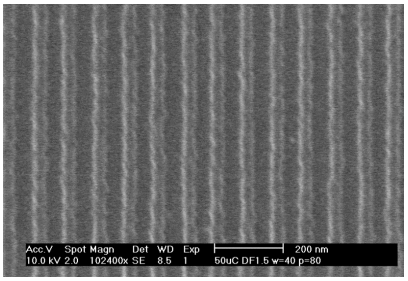

Figure 3: 40nm lines exposed with a line dose of 0.3 nC/cm at 30 kV

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CONTROL OF A SINGLE-BOND CLEAVAGE WITH MODE-SPECIFIC STRATEGIES

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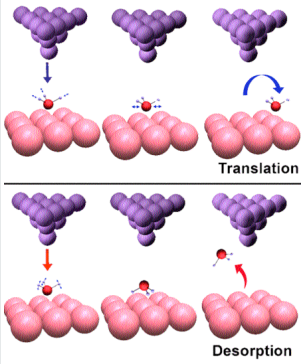
A major goal in modern chemistry is the active control of chemical reactions. Mode-selective chemistry establishes a control strategy based on the excitation of molecular vibrations to localise energy on specific reaction coordinates. Laser pulses have been traditionally used to excite specific molecular bonds and modify the reaction product branching ratio. On gas phase, for example, this strategy succeeded to control the product ratio in the dissociation of partially deuterated water (HDO) by selectively exciting the OH or the OD bonds [1].

On adsorbate systems, mode-selective strategies do more difficultly apply, generally due to the larger vibrational damping rate via coupling with surface electronic excitations, on the one hand, and to enhanced anharmonicities of the adsorbate system, on the other, which lead to a quick redistribution of the vibrational energy.

A single molecule approach to study vibrational mediated dynamics has the advantage of allowing the induction of a reaction with very low power, which allows highly sensitive detection of reaction outcome in the absence of vibrational heating or resonant heating. Molecular vibrations are excited by tunnelling electrons emitted from a scanning tunnelling tip, after they interact inelastically with the adsorbate [2]. These vibrations may provide enough energy to the molecule to activate a specific chemical transformation, generally being a bond cleavage [3].

Our investigations on a model adsorbate system, NH_3 on Cu(100), revealed that the excitation of ammonium internal modes activates the rupture of the adsorption bond, leading to the disappearance of the molecule from the tunnel junction. Intriguingly, we found that the result of this bond-cleavage was either the molecular translation along energy barriers for diffusion, or the molecular desorption, thus implying movement in the perpendicular coordinate. Each pathway involved a different number of electronic excitations, and was activated by a different molecular mode: translation was activated by excitation of N-H stretch mode, while desorption was mediated by several consecutive excitations of the N-H_3 symmetric bending (or umbrella) mode. So, the induction of ammonium motion mediated by vibrations is mode-specific.



Two pathways describing the movement of the ammonia molecule. The translation is activated by the excitation of N-H stretch modes, and this energy transferred to translational modes. The desorption is activated by the N-H_3 bending mode.

The figure above describes each of the two reaction pathways found in our experiment. In spite of being an adsorbate system, our findings indicate that the vibrational energy released into the molecule may follow damping mechanisms involving internal coupling between vibrations, on the one hand, or can be accumulated in one mode until a certain activation barrier is overcome, on the other.

Beyond the manipulation of single molecules with the STM, this single-molecule chemistry approach will certainly resolve manipulation strategies to be applied by photochemistry techniques to control and enhance the course of catalytical reactions.

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FABRICATION OF HIGH PERFORMANCE CARBON NANOTUBES BASED FETS FOR INTEGRATED CIRCUIT DEVICES

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Since their discovery in 1991 by Ijima[i], carbon nanotubes have generated great interest and research studies. In particular single wall carbon nanotubes (SWNTs) exist as semiconducting or metallic wires. They have been used to demonstrate molecular devices like transistors, diodes or SET. The recent demonstrations of room temperature SET[ii], and of SWNT transistors showing gain above unity[iii] was immediately applied to the realization of logic gates with a lateral channel extension reduced to 1 nm[iv],[v]. However these demonstrations are still based on a random deposition of nanotubes on a substrate. In order to reliably obtain large number of nanotube FETs, an efficient assembly strategy must be developed.

In this talk we are presenting two techniques which allows to reliably produce CNT transistor integrated circuit:

1.The first one is based on the local functionalisation by self-assembled monolayers (SAMs) modifying the surface properties of a prepatterned substrate. This in turn affects the interactions between the sidewalls of a CNT and the surface so that the CNTs are preferentially attracted and bonded there. This kind of technique has already been proposed in the literature, relying respectively on a local chemical functionalisation of the surface[viii] or on an electrostatic anchoring of surfactant covered NTs on amino-silane functionalised surfaces[ix]. However, the yield obtained by the processes used in these reports was not effective for the realization of large scale ICs. Using SWNTs dispersion in organic solvant and deposition on optimised SAM, we achieved highly selective deposition of high density isolated SWNTs in predefined areas of the substrate. In this presentation, we will describe the principal steps of our deposition technique and present results for self-assembled deposition of nanotubes on pre-patterned substrates. Then, we will report about the performances of such fabricated CNTFETs. We will also report first demonstration of CNTFET arrays (see figure 1).

2.The second one is based on CVD patterned growth. The Low Pressure CVD technique allowed us to produce high quality carbon nanotubes directly on a prepatterned surface. We will present briefly the growth technique which has been used and the pre and post growth fabrication process. We will finally report locally growth carbon nanotubes based transistors characteristics.

This work has been supported by the European contract IST-1999-10593 SATURN

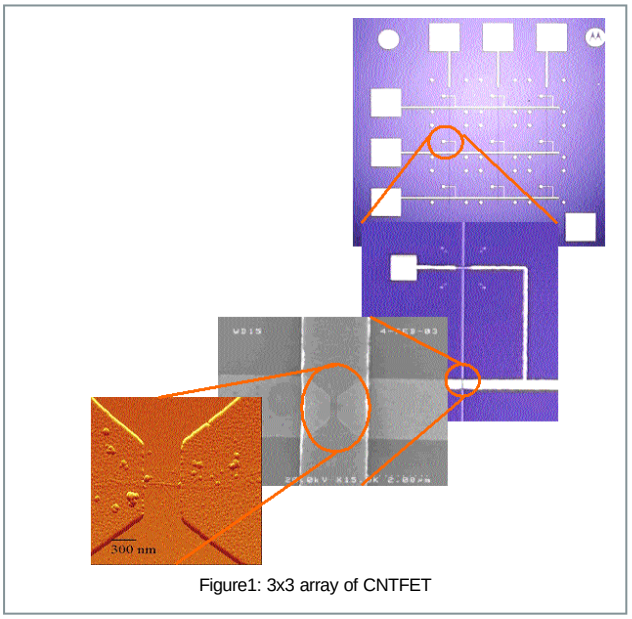

Figure1: 3x3 array of CNTFET

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25 YEARS OF METALLIC SUPERLATTICES

Phantoms

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The field of Metallic Superlattices started more or less 25 years ago with the possibility of growing structurally coherent, lattice mismatched metallic superlattices. In this short period of time, this field has experienced a virtual explosion in basic research studies in magnetism, superconductivity and mechanical properties This gave origin to a large number of unpredicted applications in a variety of fields including storage, sensors and long wavelength X-ray and neutron optics. This shows that curiosity driven basic research produces applications in the most unexpected ways.

Interesting physical properties are observed when one or more dimensions of the material cross over an interesting physical length scale such as the superconducting correlation length, the magnetic dipolar length, the exchange length, etc. In all cases, the physical properties are strongly affected and in many cases dominated, by structural disorder, inherently always present in artificially prepared metallic superlattices. It is precisely at these length scales where structural characterization techniques run into difficulties as shown in figure 1.

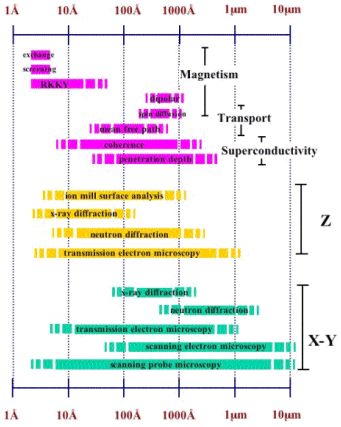

Figure 1. Physics and instrumentation length scales relevant for Metallic Superlattices. Note that the characterization length scales are different depending of the measurement direction.

Thus in order to uncover unusual phenomena which are driven by the physics of length scales, it is important to ascertain quantitatively those effects which are disorder driven. For this it is crucial to determine structural parameters quantitatively using so called refinement techniques. A very successful technique of this type is the SUPREX program which allows the use of X-ray diffraction data to obtain important structural parameters such as interdiffusion, lattice expansions and roughness. This is downloadable for free from http://ischuller.ucsd.edu.

I will describe several examples from our work in which quantitative structural studies were correlated with physical property measurements or in which structural effects cannot explain unusual physical effects observed in metallic superlattices. For instance, dimensionality and/or disorder effects in thin magnetic and superconducting layers manifest themselves by a decrease in the transition temperatures as shown in figure 2.

Interesting and unexpected dependences on roughness are found for the Giant Magnetoresistance in Fe/Cr magnetic superlattices. True superlattice effects have only been observed in very limited cases in the electronic properties of metallic superlattices. I will discuss issues which are related with the interplay of structural and

electronic length scales and the effect of these on the physical properties.

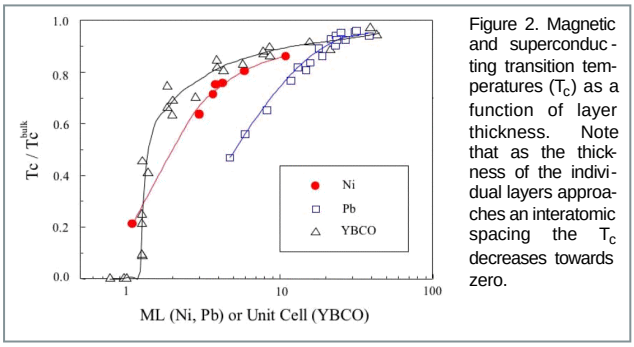

Figure 2. Magnetic and superconducting transition temperatures (T_c) as a function of layer thickness. Note that as the thickness of the individual layers approaches an interatomic spacing the T_c decreases towards zero.

In addition, I will also highlight some possible, future, new promising directions in basic research and applications in the storage, sensors and optics fields.

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NON-UNIVERSAL CONDUCTANCE QUANTIZATION FOR LONG QUANTUM WIRES: THE ROLE OF THE EXCHANGE INTERACTION

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The Landauer approach predicts that the two-terminal conductance of a phase coherent sample with ideal transmission is quantized in unit of $G_0=2e^2/h$ [1]. Experimentally, such conductance quantization was first successfully observed on ballistic quantum point contacts verifying the value of the Landauer resistance and the true nature of quantum modes in phasecoherent semiconductors [2,3]. Recently, Yacoby et al. [4] and also Tarucha et al. [5] have succeeded to produce quantum wires (QW) as long as 1-10 µm of extreme quality. Quite surprising, the conductance steps for these samples have constant heights $G_0 \cdot v$ with $0.5<v<1$ instead of the value v=1 predicted by the Landauer approach. In spite of the great amount of theoretical work devoted to study these systems, the experimental observation of conductance deviation has found no satisfactory explanation till date [6].

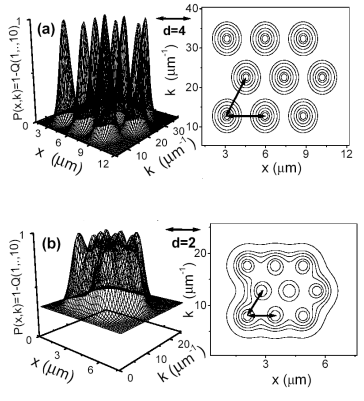

Fig 1: Exchange interaction effect due to a distribution of N=9 wave packets with different central positions, x_i, central wavevector, k_i, and identical σ_x=500nm.
P(x,k) is the probability of not finding and additional wave packet as a function of its central position, x, and wave vector, k. (a) d=4. (b) d=2. The normalized distance "d" is defined as:

$$d^2 = \frac{(k_i - k_j)^2}{2\sigma_k^2} + \frac{(x_i - x_j)^2}{2\sigma_x^2}$$

where $\sigma_k=1/\sigma_x$.

Our work shows that the nonuniversal conductance quantization can be explained as a purely Fermion exchange interaction effect. In our approach, electrons are described by wave packets and the Fermion interaction is directly introduced by assuring the antisymmetrical behavior of a wave function composed of N single-particle wave packets [7,8]. For wave packets with a large distance between them (d>2) the Pauli principle only precludes of presence of another electron around the central position of the first one (fig 1.a). In particular, we show that for a two-fermion system each electron occupies in average a phase space area equal to 2π. Therefore, the Landauer conductance step G_0 is obtained (a factor 2 for spin degeneracy is considered). However, for wave packet with a smaller normalized distance, the Pauli principle provides distributions of wave packets with very low probability (fig 1.b). In fig. 2, we have represented the probability, P(N), of finding a distribution of N wave packets separated by a distance d. In order to obtain a many-particle wave function with $P(N) \cong 1$, wave packets must be separated roughly $d \geq 2$. As clearly seen in the inset of fig.2, for a fixed value of P(N) the wave packet separation, d, increases with N due to the partial exchange interaction between all wave packets. Therefore, a reduction of ρ, and consequently of G_0, is obtained. In fig. 3, we have plotted the conductance reduction as a function of the QW length, L. For QW shorter than 1 µm (at very low bias and temperature), one electron is present in the phase space that precludes a second electron from entering, limiting the maximum conductance to G_0. On the other hand, a reduction of G_0 is obtained, in agreement with experimental data [4], for longer samples due to active presence of many (>1) electrons inside the phase space that slightly increases the range of the Pauli exclusion interaction.

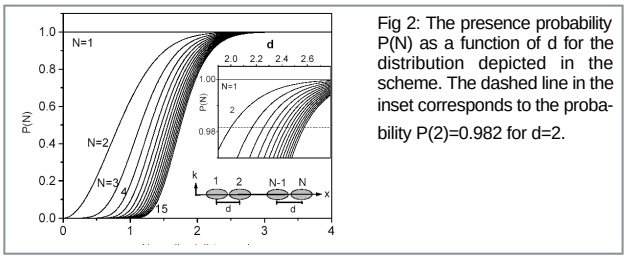

Fig 2: The presence probability P(N) as a function of d for the distribution depicted in the scheme. The dashed line in the inset corresponds to the probability P(2)=0.982 for d=2.

In conclusion, we have shown that the origin of the puzzling nonuniversal conductance quantization in long QW is ultimately due to the Pauli Exclusion Principle. A two-fermions system provides a maximum conductance equal to the well-known Landauer value G_0 and conductance reductions are obtained for many-fermions systems. Since electrons at different quantum modes do not suffer from exchange interaction, the conductance reduction is identical for each quantum mode, in agreement with experimental results [4].

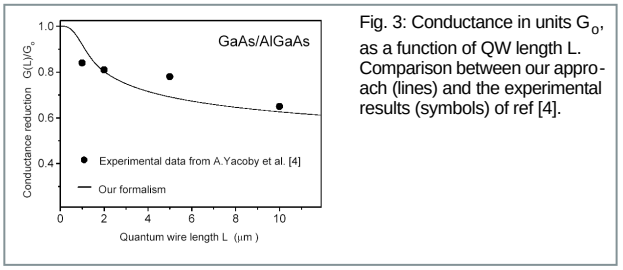

Fig. 3: Conductance in units G_0, as a function of QW length L. Comparison between our approach (lines) and the experimental results (symbols) of ref [4].

Finally, the present work is based on a novel approach (that we call the many particle wave packet formalism [8]) that provides a new framework to study quantum transport in the nowadays very active field of nanoelectronics.

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NOVEL DNA-BASED MOLECULAR NANOWIRES

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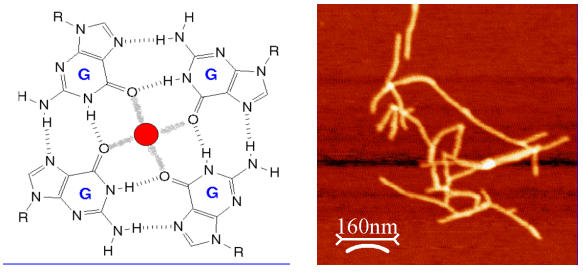
Nanoscience and Nanotechnology are emerging in the scientific community and beyond as building structures that are on the nano- rather than the micro-scale is more than just reducing their size by 1000 times. New exciting scientific questions and fascinating technological opportunities rise upon this miniaturization. Molecular Nanoelectronics that combines knowledge and expertise in physics, chemistry and biology is a leading direction in this new field, where the development of new molecular nanowires is a central theme.

DNA is one of the most attractive candidates for future molecular electronics due to the high density of its components, its accurate synthesis and its double-strand recognition properties that suggest self-assembly. Although others and we have shown by direct electrical transport measurements that some DNA sequences can indeed support electrical current,[1] it seems that DNA itself is not a good electrical molecular wire. Therefore, we develop novel modified DNA-based derivatives that may transport current in a more efficient manner. One example for such structures is the G4-DNA, a molecule composed of consecutive tetrades of guanine (G) bases. G4-DNA is a wire with and without metal ions disposed in the internal cores of the G tetrades. A linear arrangement of closely separated redox-active ions in the center line of the molecule may lead to the formation of an effective molecular wire by means of electron transfer or transport. Moreover, the unique structure of the tetrades leads to a much stronger and stiffer structure than that of the native DNA (diameter 2.1 nm), although its diameter is only 2.3 nm.



A scheme of a G4-DNA tetrad with a metal ion in the central canal (left) and an AFM image of long G4-DNA based nanowires

We have produced two different types of G4-DNA wires with length up to a few microns long with various metal ions in the central canal of the molecule. The molecules were characterized and compared to each other and to native DNA by optical methods, by AFM techniques for the morphology, by electrostatic force microscopy (EFM) for the polarizability and by direct electrical transport measurements for the electrical properties.

In this talk I will present morphological characterization, EFM and electrical measurements and possibly mechanical measurements of the new G4-DNA nanowires.

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LTSTM INVESTIGATIONS ON ULTRATHIN INSULATING FILMS: NaCl/Cu INTERFACE STATES AND ADSORPTION OF METAL ATOMS

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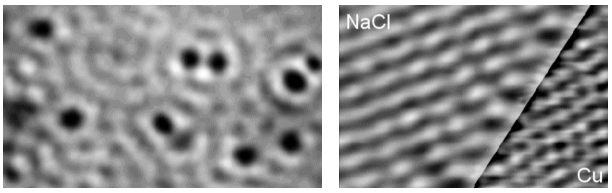
While scanning tunneling microscopy has been proven to be a powerful technique to study surfaces of conducting substrates on the atomic scale it is unfortunately not applicable to the study of bulk insulators. Ultrathin insulating films on the other hand can be grown thin enough to be studied by scanning tunneling microscopy. The high lateral resolution in combination with local electronic spectroscopy allows the study of metal/insulator interfaces down to the atomic scale. Moreover the adsorption of atoms and molecules on these films, including effects of the film strain and the image force induced by the underlying metal substrate, can be studied in detail. We have investigated 1 - 4 ML ultrathin films of NaCl epitaxially grown on different copper substrates.

On low index (111) surfaces of noble metals exists a surface state and the electrons in the surface state form a two dimensional electron gas. Scattering of the electrons in the surface state gives rise to the formation of the well known standing wave patterns [1]. It is known that these surface states survive as interface states below ordered adsorbate layers[2]. In the case of Xe/Cu(111) these interface states could be recently imaged with a LT-STM [3].

In the case of NaCl(100)/Cu(111) an interface state band descending from the surface state band of the clean Cu(111) surface is observed. In Fig. 1 typical standing wave patterns of the electrons in the interface state can be observed. Since the NaCl film is almost free of point defects, typical scattering centers are represented by impurities in the copper substrate surface. Detailed spectroscopic experiments at 8K determined the bottom of the interface band to be about 225meV below the Fermi-Level and a small increase of the effective mass of the electrons is observed. More importantly Moiré patterns arise from of the incommensurate growth of the NaCl(100) on the Cu(111) surface. This additional periodicity produces a splitting in the band structure of the interface state of about 50meV at 20-400meV above the Fermi-Level, depending on the specific rotation of the NaCl domain. Therefore interface state band shows a one dimensional band gap, that appears in the images as standing waves. These patterns cause a modulation of the potential and thereby form a 1d bandgap in the 2d interface state band. At NaCl island edges one can observe the refraction of electrons in the interface state band obeying the Snellius law of refraction (Fig.1b).



(a) 4.5×10^{-10}Å; -20mV; 230Å×190Å (b) dI/dV image; 53mV; 200Å×130Å

Fig. 1: a) Standing wave patterns can be observed on NaCl(100)/Cu(111). b) At NaCl island edges the electrons are refracted

The ultrathin NaCl films have been used as substrate to investigate the adsorption of single metal atoms and metal dimers. The binding sites of Cu, Ag, Au and Pd were determined, local spectroscopy performed and atomic manipulation processes were studied.

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INTEGRATING LOGIC FUNCTIONS INSIDE A SINGLE MOLECULE

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In molecular electronics one can adopt several different strategies towards the implementation of logic functions into molecules [1]. The most natural one seems to be an electrical circuit approach, since current circuit design concepts in semiconductor technology are based on it [2]. However, our recent work has demonstrated the problems faced by this approach [3],[4]. While large hybrid-molecular architectures can be designed in principle, they are not able to compete with current CMOS technology due to the restrictions on bandwidth and size imposed by the interface between the active molecule and the metallic grid [3]. Major difficulties will be encountered when scaling down such architectures to mono-molecular architectures because of fundamental differences between the Boltzman electron transport regime, in which CMOS electronics operates and the ballistic or tunneling regime of transport [4].

As a consequence of these difficulties a new architectural concept which makes use of the specific properties of electron transfer phenomena inside a molecule has been developed [5]. It takes into account the influence that symmetry has on electron transmission through highly delocalised π-states of an aromatic molecule and uses this dependency of charge transport on molecular geometry for storing information. In this paper we present an extension of this concept to information processing, where the aim is to implement logic functions inside a single molecule. Fig. 1 shows intra-molecular XOR- and AND-gates, where the transmission coefficients have been calculated with the Elastic Scattering Quantum Chemistry (ESQC) technique [6]. For these calculations the molecular orbitals have been described within the extended Hückel approximation taking full account of the details of their three-dimensional structure. The input is fed into the system by rotating nitro-groups, the output is read as the current being transferred between a reference and a measurement electrode. Our paper also investigates ways for integrating both logic gates into the same molecule, which would provide a half-adder inside a single molecule.

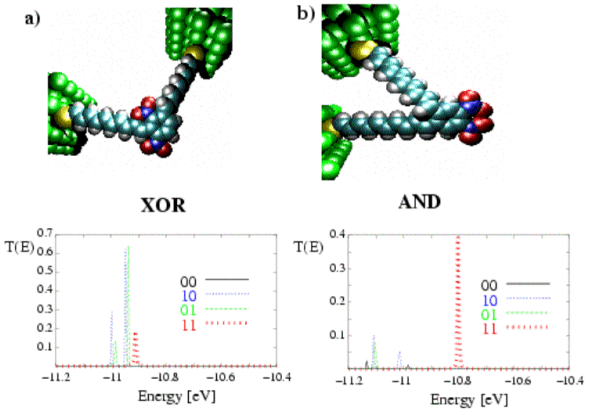

Fig. 1: A benzene molecule is connected to two gold electrodes by sulfur atoms and polyacetylene wires and the transmission through the molecule can be designed to have the characteristics of either a) a XOR-gate or b) an AND-gate. The type of gate is defined by the positions on the benzene ring, where the wires are connected, namely in a meta-configuration for the XOR-gate and in an ortho-configuration for the AND-gate. It is also crucial on which ring positions the nitro-groups are bonded to the molecules. They are rotated for defining the input, where the substituents interact with the π electrons of the benzene ring, when they are planar to the ring and there is no interaction when their rotational state is perpendicular to the benzene molecule.

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LOCAL CHARACTERIZATION OF ELECTRON TRANSPORT PROPERTIES IN MULTIWALLED CARBON NANOTUBES

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As one seeks to lower the dimensions of electrical circuits there are problems with overheating in metal wires. Conventional metal wires can only take about 10^4 A/cm^2 until the resistive heating becomes a problem. Using thin film conductors deposited onto heat sinks can circumvent this, and current densities of up to

10^7 A/cm^2 can be reached without immediate breakage. At these high current densities an another problem emerges, the electromigration.
As the electrons scatter against defects in a conductor there is a net force on the defects and they begin to migrate, leading eventually to circuit failure. Here carbon nanotubes can make an important difference as they are predicted to be ballistic conductors, i.e. the electrons travel freely along the tubes without any scattering. For an ideal tube with good electrical contacts at both ends one would therefore expect to have a conductance of twice the quantum conductance G_0 ($G_0 = 2e^2/h \cong 1/13$ (kΩ)-1). This would give a total resistance of around 6.5 kΩ through a nanotube including its contacts (independent on the length of the tube). In practice such perfect tubes are both hard to produce and to make good contacts to, and several studies have reported diffusive conduction in lithography connected multiwalled carbon nanotubes (MWNTs) [1,2]. Quantum conductance have only been observed at room temperature for suspended MWNTs (produced using the pure carbon arc method) after multiple dipping into a liquid metal [3]. The observed conductance was around G_0, rather than $2G_0$, but nearly independent of the submersion depth. It was concluded that ballistic conduction occurs in undoped and undamaged tubes for which the top layer is metallic and the second layer semiconducting [3]. Catalytically grown MWNTs are highly defective and would therefore not display any ballistic transport.

Here we report studies on suspended MWNTs filled with iron. We have recently developed an instrument combining scanning probe microscopy (SPM) with transmission tunneling microscopy (TEM) [4,5]. Using this we have the unique ability to make electrical contacts with suspended carbon nanotubes and to measure the electrical conductance at selected positions (see figure 1). The MWNTs were made by pyrolysis of ferrocene and subsequently attached to a sample using conducting epoxy glue. Sonification or any further cleaning of the tubes was avoided in order to minimize structural damage of the tubes.

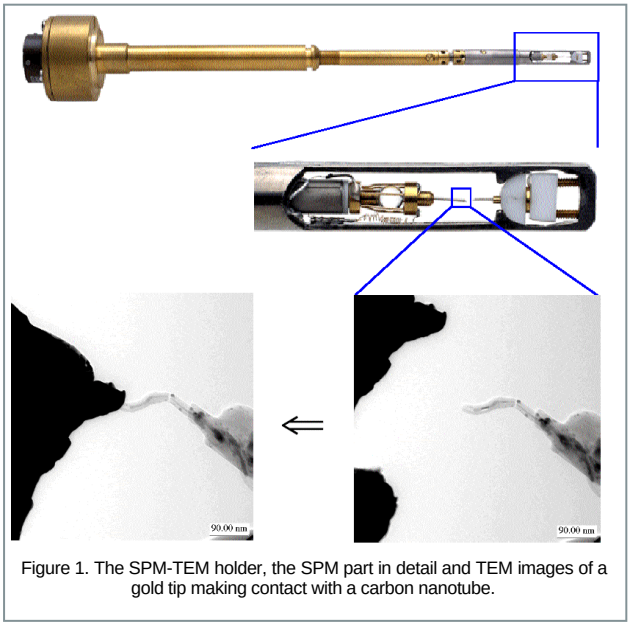

Figure 1. The SPM-TEM holder, the SPM part in detail and TEM images of a gold tip making contact with a carbon nanotube.

By contacting individual tubes inside the TEM, with an Au tip, we find an overall conductance around G_0 at low biases (see figure 2). The conductance increases with the applied bias up to values above $2G_0$ for the differential conductance. This is similar to earlier observations and has been attributed to the increase in the density-of-states in a metallic nanotube above the energy gap [3]. The TEM images reveal a number of defects in the tubes and conductance measurements at various positions along the tubes indicate diffusive rather than ballistic conduction. In spite of this the tubes can withstand very high current densities, up to 10^8 A/cm^2, before rupture begins. This seems promising for applications of catalytically grown nanotubes as these can be manufactured in place as opposed to arc-discharge grown ones.

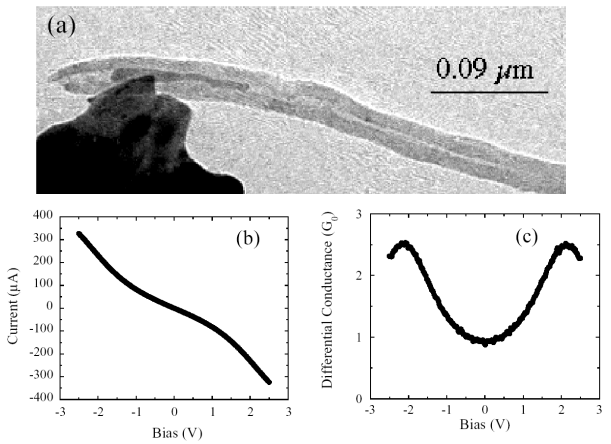

Figure 2. TEM image of the movable tip in contact with a carbon nanotube (a), corresponding I/V curve (b) and differential conductance (c).

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FABRICATION OF NANODEVICES WITH SUB 10nm SCALE FOR TRANSPORT EXPERIMENTS ON MOLECULES

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Molecular rectifier can represent the building blocks of a different type of electronics based on organic molecules rather than conventional solid state semiconductors. The typical size of a single molecule is of the order of a few nanometers; thus is required to fabricate devices with metal electrodes separated by a nanometer-scale channel. In this work, we report about fabrication of two and three-terminal nano-devices consisting of metal (Cr/Au, Ti/Au or Ti/Pt) tip-shaped electrodes on Si/SiO_2 , with tip separation between 100 and less than 10 nm, and of Ag control electrode on the back of Si substrate. Standard EBL process allowed us to obtain nanotips with separation not smaller than 40 nm according with CAD circuit design. In order to obtain tip separation smaller than 40nm up to 10 nm, before the EBL process, we used the defocused e-beam to brush the PMMA layer for a precise time (from 10 to 50 sec) (fig.1). The smallest distance between tips (less than 10nm) is obtained combining standard EBL and lift-off followed by

Au electroplating deposition in order to reduce the initial gap of 100nm up to a minimum of 7±2 nm (fig.2) . The fabricated nanodevices are inspected by plan-view scanning electron microscopy (SEM) to establish the success of the whole technological process. Successively all nanotips were electrically characterized by I/V measurements in order to make sure of their possible use as probes of molecular conduction. In a typical I-V measurement of an "open-circuit" nanodevice, no significant current is observed (current range -10±10 pA, resistance ≅1TW) confirming the success of the process. The succeeded nanodevices are used for transport experiments in molecules placed by RT cast deposition between electrodes (fig.3). After the molecule deposition and the electrical characterisation, the devices are observed by atomic force microscopy and SEM in order to evaluate the possible damage and morphological changes of the planar nanotips and of active molecular layer.

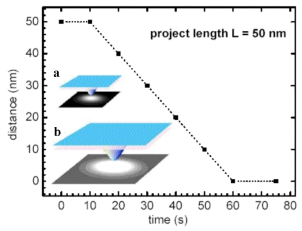
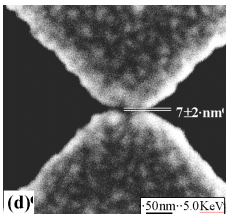


Fig. 1: Reduction of separation between electrodes as function of time Δt of PMMA brushing by a defocused e-beam.

Fig. 2 SEM image of electrodes obtained with EBL and lift-off followed by Au electroplating deposition.



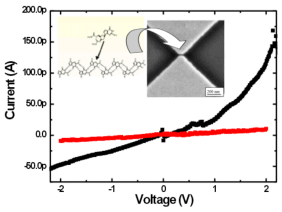


Fig. 3: I/V characteristics of molecular device with inter-electrode separation of 20nm. The open-circuit current (nanotips without molecule, red line) stays in the range -10±10 pA, much lower than the molecular response (black line).

DEPOSITION AND NANOPATTERNING OF MN12 SINGLE-MOLECULE MAGNETS ON SURFACES WITH SIZE AND POSITIONAL CONTROL AT MULTIPLE LENGTH SCALES

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Single-molecule magnets (SMM) have a large high-spin ground state with appreciable magnetic anisotropy, resulting in a barrier for the spin reversal. As a consequence, interesting magnetic properties such as out-of-phase ac magnetic susceptibility signals and stepwise magnetization hysteresis loops, due to individual molecules rather than to long-range ordering; are observed[1]. Such molecules may become materials with a potential impact in ultra-high density magnetic storage, provided they can be organized into addressable domains. With this aim, it has been recently demonstrated the possibility to deposit very small clusters, possibly made of single molecules, onto a polycarbonate surface[2]. Self-assembly of thiol-substituted Mn_{12} clusters have also been achieved on Au thin films[3]. In both cases, no control of position and distance was shown, and despite the latter method is amenable for contact printing, it may be desirable to devise patterning of molecular magnets onto a variety of surfaces beyond gold with size and positional control.

Here we present two methods based on unconventional parallel nanolithography for patterning Mn_{12} single-molecule magnets on a large area and with nanometer resolution on surfaces with different nature. The first method uses a stamp-controlled deposition of molecules from a solution and exploits competing interactions between the molecules and the substrate. The second method permits the fabrication at a submicron resolution of an ordered pattern of Mn_{12} single-molecule magnets dispersed in a polycarbonate matrix by a modified micro-transfer molding with a subsequent solvent exposure.

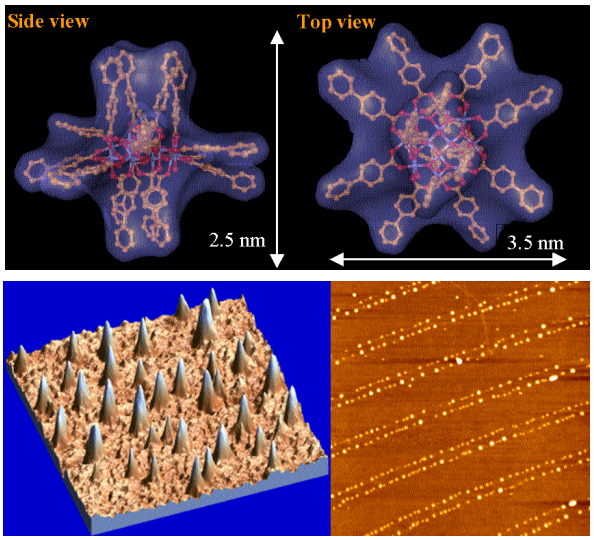

Figure. Top: Views of a Mn_{12} single-molecule magnet showing its size. Bottom, left: AFM image of such isolated Mn_{12} single-molecule magnets on the surface of a polycarbonate polymeric thin film. Bottom, right: Nano-droplets of such Mn_{12} single-molecule magnets printed by stamp-directed self-organization. Droplets are a few nm high, 70 nm FWHM, 130 nm apart along the line.

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Short Scientific Visits Funded by Phantoms

Report 1

GOAL: Find the saturation magnetization and its temperature dependence between 5 to 300 K for γ´Fe_4N epitaxial films. This information, together with high temperature data, allows the determination of the magnetic moment per Fe and the Curie temperature, proportional to the strength of the exchange interaction in these new materials.

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Laboratory visited: Prof. KV Rao, research leader, "Division of Material Physics, Department of Materials Science and Engineering, Inst. Material Vetenskap Avd. Teknisk Material Fysik (Tmfy-MSE, KTH), Royal Institute of Technology", SE 10044 Stockholm, Sweden
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Duration of the visit: October 30 to November 5, 2003

Magnetic properties from 5 to 300K of epitaxial γ´Fe_4N films

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During the past decades, iron nitride compounds were extensively investigated due to their excellent magnetic properties, which make them suitable for applications in high density magnetic storage devices. All iron nitrides are metallic conductors and metastable with respect to decomposition in Fe+N_2. The decomposition is limited by kinetic barriers. Among the ferromagnetic nitrides, γ'Fe_4N phase is of special interest. This nitride has a cubic structure, contains 20 at.% N and is stable at temperatures below 400ºC. The saturation magnetization, M_S was reported to be between 1.8 T and 1.9 T. {1,2,3}.

Up to now, polycrystalline thin films of γFe_4N were grown on (111) Si substrates by ion beam assisted evaporation\cite{4} and reactive sputtering in a NH_3 atmosphere.{1} With N_2 as reactive gas in a dc magnetron sputtering facility, epitaxial γ'Fe_4N films were grown on (001) Si substrates with a (002) Ag underlayer, as claimed by Brewer et all.{5} Concerning purity, crystal quality, roughness or magnetic properties, no details were reported.

Recently, the interest in iron nitrides has also increased due to the possibility of developing an all-nitride epitaxial magnetic tunnel junction with γ'Fe_4N as magnetic electrodes and epitaxial Cu_3N as insulating barriers.{6} The intermixing at the interface, commonly observed at metal/metal interfaces, may be reduced due to the Fe-N and Cu-N bonding.

Up until now, the lack of high quality epitaxial γFe_4N films made impossible a thorough investigation of the magnetic properties of this phase. However, rather recently {7,8}, such high quality epitaxial film has been grown by molecular beam epitaxy of iron in the presence of atomic nitrogen as obtained from an rf atomic source.

The measurements described in what follows are complementary to X-ray, Mössbauer, detailed Kerr Magneto Optic (MO) measurements, anisotropy determination by MO torque and domain observations at RT{9}

The activities developed during José Luis Costa Krämer trip to Tmfy-MSE, KTH concentrate on the SQUID (Quantum Design $MPMS_2$ system) measurements of the magnetic properties of γ´ Fe_4N single crystal grown on MgO substrates. The film used was 200 Å thick, with a Cu protective capping layer. This material is a strong candidate to be part of Ferromagnetic Tunnel Junctions with applications as Magnetic memories MRAM and logic. The possibility of growing the whole tunnel junction structure by alternatively depositing Fe and Cu in a Nitrogen atmosphere makes this system very attractive for industrial MRAM production. This is so because Cu_3N has good insulating properties.

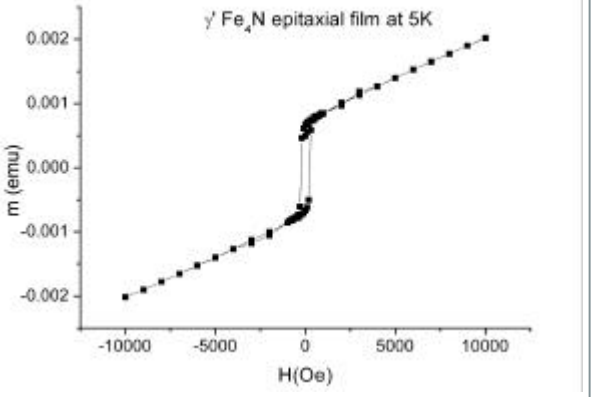

Fig. 1 Hysteresis Loop of a γ'Fe_4N single crystal film grown on MgO and capped with a copper layer measured at 5K

The measurements -carried out with Amita Gupta- focus on the estimation of the saturation magnetization of the material, and its temperature dependence, trying to obtain an estimation as well of the Curie temperature. This is somehow a difficult task, since nitrogen tends to diffuse away at moderate temperatures, between 300 and 400 ºC. The first measurements, Fig.1, a hysteresis loop at 5K with the field applied parallel to the film plane, revealed a low field hysteretic behavior plus a paramagnetic kind of contribution of unknown origin. The saturation magnetization derived from this loop and the lateral dimensions of the loop and the thickness deter-

mined by low angle X-ray measurements is of about 1.85 T {9}.

In order to ascertain the possible origin of this behavior we perform magnetization versus temperature curves at three fields, 0, 100 and 1000 Oe (Fig.2) and hysteresis loops at three more temperatures, 100, 200 & 300 K (Fig.3). This paramagnetic contribution could not be explained by the magnetic properties of the substrate (MgO is diamagnetic) or the capping layer, (Copper is diamagnetic as well).

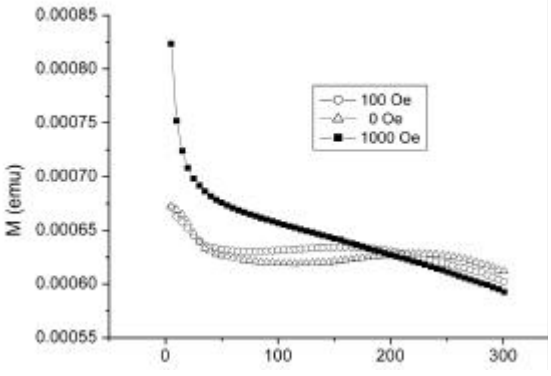

Fig. 2 Magnetization versus temperature at 0, 100 and 1000 Oe for a γ/Fe_4N single crystal film grown on MgO and capped with a copper layer

As observed, and comparing with the loop at 5K shown in Fig. 1, as the temperature is increased the paramagnetic component at large fields disappears turning into the expected diamagnetic component arising from the substrate. In parallel, the coercivity of the film decreases as the temperature is raised as expected.

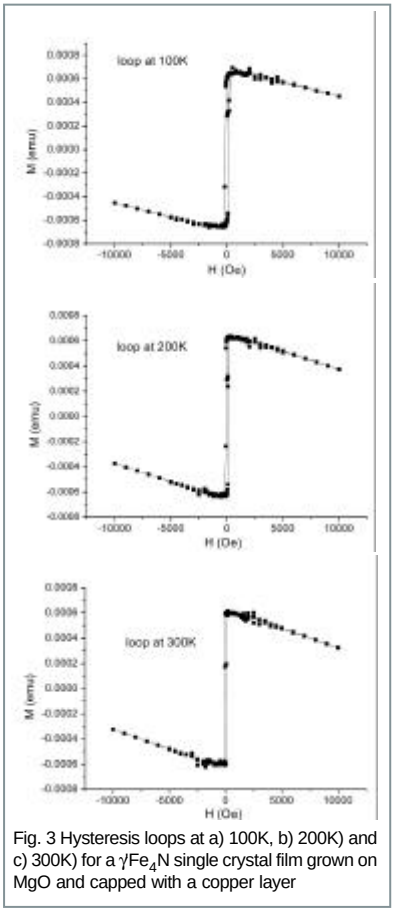

Fig. 3 Hysteresis loops at a) 100K, b) 200K) and c) 300K) for a γ/Fe_4N single crystal film grown on MgO and capped with a copper layer

In order to clarify the possible origin of this extra magnetic term, the film was removed from the SQUID, and cleaned thoroughly of possible remains of high temperature cement used in previous measurements. This cement in the rear part of the MgO substrate is known not to give any magnetic signal in VSM measurements between 300 and 800 ºC. However, the cement material could have magnetic transitions at low temperatures explaining the measured behaviour. The cement was removed by polishing the rear part of the MgO substrate gently, blowing dust remains, and washing in alcohol. After this the film was introduced again in the SQUID.

A hysteresis loop at 5K and a remanent magnetization versus field at zero field were measured. These are shown in Fig. 4 and 5 respectively.

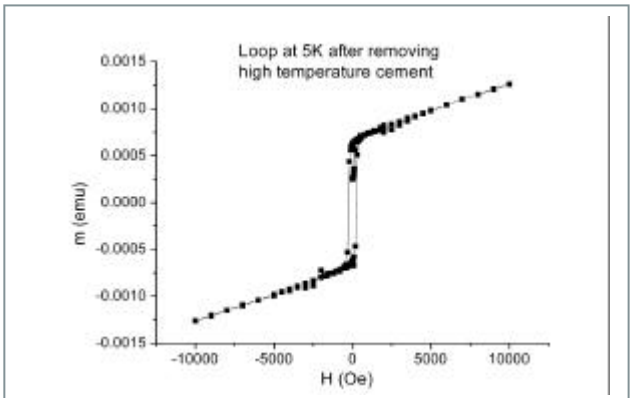

Fig. 4 Hysteresis Loop of a γ' Fe_4N single crystal film grown on MgO and capped with a copper layer measured at 5K. As compared to Fig. 1 the film has been cleaned of possible remains of high temperature cement used in previous measurements.

Notice that after removing the high temperature cement, the linear positive (paramagnetic like) component of the magnetization has been reduced. However, the overall behavior of the magnetization, and its temperature dependencies are basically the same. These facts open interesting questions about the role of the anisotropy and magnetic interactions in the low temperature behaviour of iron nitride single crystals. These effects have been observed both for Cu capped and Cu_3N capped films, pointing out to something intrinsic to the film magnetic properties. A recent paper {10} has also observed this behaviour, although it has attribute it to the formation of a ferrihydrite phase in the film, which seems unlikely in our case due to the presence of a protective capping layer. Our film will be further studied by cycling temperatures, (ZFC & FC dependencies) and ac susceptibility at low temperatures, trying to discern the magnetization processes and spin structures at low temperatures, responsible of the anomalous magnetization dependencies.

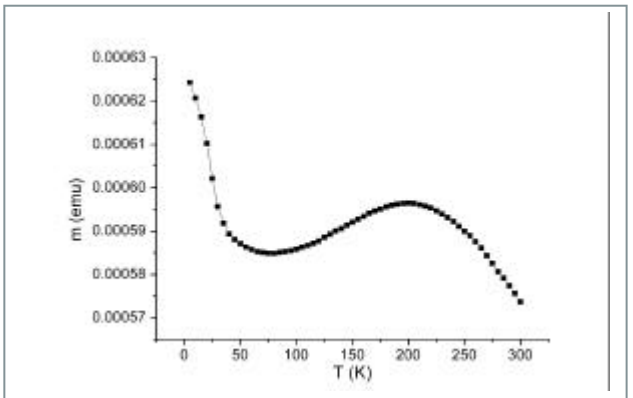

Fig. 5 Remanent magnetization versus temperature at 0 a $\gamma'$$Fe_4N$ single crystal film grown on MgO and capped with a copper layer

Summary: Both the saturation magnetization and its temperature dependence have been measured between 5 to 300 K for a γ' Fe_4N epitaxial film. These data is used to determine the magnetic moment per Fe and the Curie temperature, proportional to the strength of the exchange interaction in these new materials. The low temperature data presents some anomalies (deviations from a decay α $T^{3/2}$ law) that will be further studied by ac susceptibility.

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Acknowledgements

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Thin films were grown by D.M.Borsa (D.O. Boerma group).

Report 2

GOAL: Work in the problem of ionic shell in metallic nanocontacts.

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Duration of the visit: September 02-15, 2002

Ionic Shell and Subshell structures in metallic nanocontacts

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Recently it has been observed that the stability of alkali metallic nanowires is influenced by electronic shell filling effects [1]. However for increasing nanowire diameters there is a crossover towards crystalline wires with shell closings corresponding to the completion of additional atomic layers [2]. These shell structures are a close analog of the shell structures observed for metal clusters [3]. In fact, for metal clusters it was observed that clusters with certain "magic numbers" of atoms are more stable than others. Alkali and noble metal clusters are well described by jellium theories where the fluctuations in the electronic energy play a dominant role, while in other metals as Aluminum, the shell behavior is due to the fluctuations in the atomic energy. In the present work we have been interested in this kind of phenomenon but in other metals different to alkali ones.

A custom made scanning tunnelling microscope (STM) was used to form and break the contact between two metallic polycrystalline electrodes (Al or Au). We have accomplished conductance G measurements at room temperature for Au and Al nanocontacts under ambient conditions and obtained conductance histograms for both cases. For Au we also performed experiments in presence of parafinic oil and confirmed that gold conductance histograms do not depend on the environment [4]. The experimental conductance histogram for Au is depicted in Fig. 1. In order to determine the electronic or atomic origin of the peaked structure seen in Fig. 1, we proceed as described in References [1,2]. We have determined the position of those conductance values where the histogram presents maximum values (i.e. the conductance histogram peaks). We have assigned to each conductance peak an index m. Finally we analyze the behavior of $(G/G_0)^{1/2}$ versus the peak number m (G_0 is the quantum conductance unit $2e^2/h$). The inset of Fig. 1 shows such resulting curve for the Au case, as extracted directly from the histogram. Applying the same reasoning followed in References [1,2] the presence of electronic or ionic effects governing the appearance of more stable configurations are associated to different slopes in the $(G/G_0)^{1/2}$ versus m curves. In the present study, our results show electronic shell filling effects at low conductance ($g^{1/2}$ ~ 0.46m) and ionic subshell effect for high conductance($G/G_0^{1/2}$~0.21m). That is, we demonstrate that there is a crossover from electronic to ionic behavior in gold at room temperatures in a similar way to the behavior seen in alkali metals at lower temperatures.

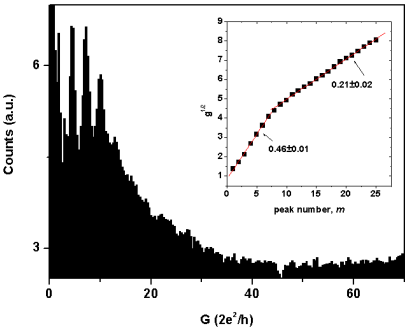

Fig. 1. Experimental Au conductance histogram H(G) at room temperature. The inset shows $(g=G/G_0)^{1/2}$ vs. the peak number index m.

In order to understand more in detail the different regimes observed in experiments, we performed simulations of the minimum cross-section histograms of breaking Al and Au nanocontacts. For this we used the Molecular Dynamics (MD) technique, and used the state-of-the-art many-body EAM interatomic potentials for Al and Au. This EAM potentials are able to fit many bulk and surface properties [5]. As a starting point of our MD simulation we

consider a parallelepiped supercell containing more than thousand atoms ordered according to a fcc crystallographic structure. Two bi-layer slabs are frozen during subsequent MD stages, defining the bulk support (electrodes) of the nanocontact during the breaking process. Then the nanowire is stretched by separating both supporting frozen slabs at a constant velocity. The evolution of atomic positions during the elongation process allows us to know the changes of the nanocontact geometry, and evaluate the time evolution of the minimum cross-section S_N (in units of numbers of atoms) as explained in Ref. [6]. More details of our simulations can be find elsewhere [7]. An example of nanocontact stretching is depicted in Fig. 2a. In Fig. 2b we show the evolution of S_N as a function of the nanocontact elongation for four different realizations. Under the semiclassical Sharvin approach, it is easy to relate the nanocontact section with the conductance ($G \sim S_N$) [9] and therefore the conductance histogram and the minimum-cross sections histograms are identical except for a scale factor. Following a procedure similar to that used to construct H(G) (i.e., by accumulating S_N traces) we construct minimum cross-section histograms $H(S_N)$. The number of single nanowire breaking realizations considered is such that the obtained relative histogram peak structures are unchanged under further averaging (see Fig. 2c). We have shown the good agreement between simulations and experiments for Al histograms in ref. [8]. We also performed such kind of simulations for Au nanocontacts at room temperature. Then, from the resulting histograms, we computed the corresponding conductance G using the Sharvin approximation [9].

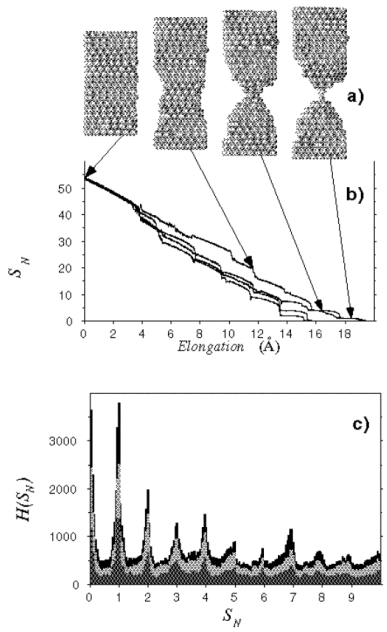

Fig. 2. (a) Typical nanocontact configurations during the elongation of the sample. (b) Minimum cross-section S_N evolution for four different Al nanowires. The arrows indicate the corresponding S_N for each configuration. (c) Minimum cross-section histograms $H(S_N)$. Dark gray and black curves correspond to histograms obtained with different number of realizations (35, 70 and 100, respectively).

Finally we plotted $(G/G_0)^{1/2}$ versus the corresponding peak number m in order to study the ionic shell and subshell structure of nanocontacts as performed in refs. [1,2] for alkali metals.

In Fig. 3 we present comparison between the $(G/G_0)^{1/2}$ curves of simulations (open symbols) and experiments (black symbols) for both cases, Au and Al, at room temperature. The agreement between experiments and simulatuions is remarkable, excluding large conductance values for the reasons we will discuss below. An advantage of the simulation is that we can go to higher conductance values than we have experimentally explored. Nevertheless, for large diameter wires the detailed peak structure observed at intermediate conductance values (ionic subshell signature) is unresolved in simulations. In other words, the typical broader maxima obtained in simulations, evidencing complete ionic shells, obscure details of the peak structure corresponding to subshells observed in the Au and Al experimental histogram. In fact, the high slope at large conductance values (see Fig. 3) agrees well with that expected for complete shells for the octagonal candidate crystalline structure [10].

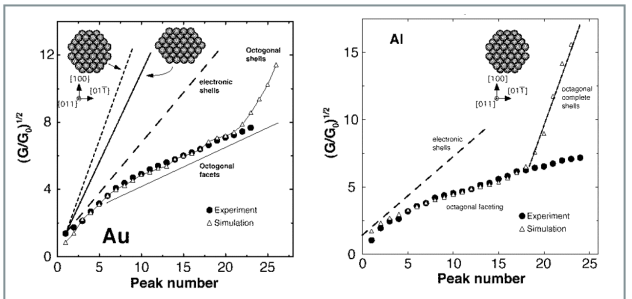

Fig. 3. Comparison between simulations and experiments of $(G/G_0)^{1/2}$ versus the peak number curves for Au and Al. The different slopes correspond to different regimes as indicated in the figures.

In conclusion, we believe that these studies consolidate conductance histograms as a new powerful tool for the study of the stable configurations of nanostructures and the determination of the corresponding magic numbers. More information about this work can be find elsewhere [11,12].

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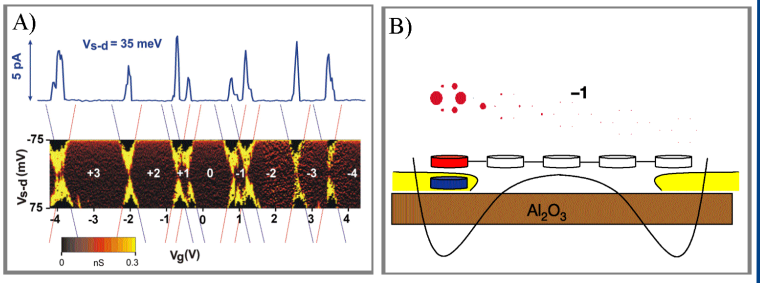
Scientific Paper Highlights

Single electron transistor of a single organic molecule with access to several redox states A single p-phenylenevinylene oligomer molecule was placed in a nanogap between the source and drain electrodes and the electron transport through this system was studied as a function of voltage on the third electrode serving as an electrostatic gate. In these experiments the electronic levels of a single π-conjugated molecule in several distinct charged states control the transport properties of the device. Comparison between the intrinsic (redox) addition energies of the molecule in solution and those measured in the SET reveals a strong perturbation of the molecular properties. A very significant reduction of the gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital has been observed. This surprising effect could be caused by image charges generated in the source and drain electrodes resulting in a strong localization of the charges on the molecule, as supported by simple model calculations and recent spectroscopic studies.
The results show that the molecule cannot be conceptually separated from the electrodes due to these electrostatic image charge effects, even when the electronic overlap between the electrodes and the molecule is weak, as shown by the observation of single-electron tunneling phenomena. These effects must be taken into account when designing molecules to be used in solid state devices.



A) Measurements of the device differential conductance as function of source-drain and gate voltages. The full solid line at the top of the figure shows a representative current trace as a function of gate voltage (T = 4.2 K).
B) Schematic view of the molecular transistor and a charge distribution calculated by a Hubbard model for a single charge trapped on the molecule and stabilized by its image; the size of the red circles is proportional to the atomic charge density.

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- Mattias Hjort (Dept. of Chemistry, The University of Arizona, Tucson, Arizona 85721-0041, USA).
- Jérôme Cornil, Jean-Luc Brédas (Lab. for Chemistry of Novel Materials, Center for Research in Molecular Electronics and Photonics, Univ. of Mons-Hainaut, Mons, Belgium).
- Nicolai Stuhr-Hansen, Per Hedegård and Thomas Bjørnholm (Nano-Science Center, Dept. of Chemistry and Niels Bohr Inst., Univ. of Copenhagen, Copenhagen, Denmark).

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Nature (Vol. 425, October 2003, p. 698)

Conductivity of Single Molecules The interconnection of nanoscale objects is of great importance for the construction of circuit elements by chemical means and one of the current difficulties is how to measure the electrical conductivity of possible molecular wires.

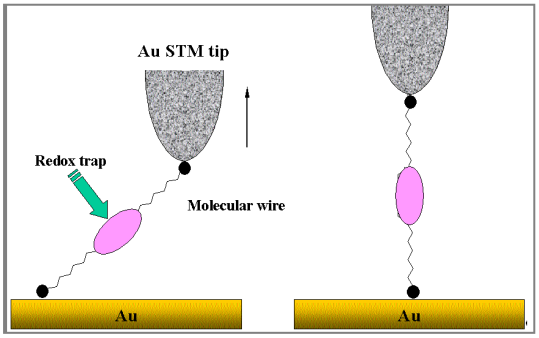

Figure 1 Schematic representation of the stretching of a molecular wire employing an STM tip. The molecular wire contains two terminal thiol groups that are used to attach the molecule to the tip and the substrate. The redox centre acts as a switching element of the wire and electron injection leads to an increase of conductivity

It is known now that the measured conductivity is greatly affected by the formation of chemical contacts at both ends of the molecular wire. For this reason, a combination of thiol chemistry and scanning tunnelling microscopy has been developed at the Centre for Nanoscale Science at Liverpool University to carry out these measurements.[1] A schematic diagram of the method is shown in Figure 1. A low surface concentration of a dithiol is placed on a gold surface. When a gold STM tip approaches the surface, attachment of one end of the "wire" to the tip takes place. This manifests itself by a current-distance dependence very different from that in the absence of the "wire" connecting the surface and the tip. As the molecular wire is extended, the currents observed correspond only to conduction through the molecule in the gap, thus allowing a calculation of molecular conductivity. Conductivity measurements can be made even in aqueous solutions, thus allowing the measurement of conductivity changes induced by a change in the redox state of the molecule under consideration.

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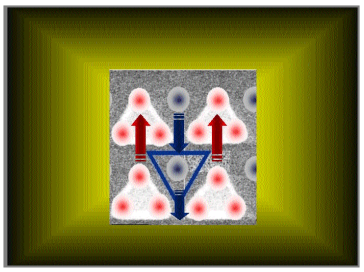
Journal of the American Chemical Society (2003)

Scientific Paper Highlights

A new nanodevice: A superconducting reversible rectifier J. E. Villegas et al. reported in the 14 of November issue of Science (Science 302, 1188, 2003) a new promising device; that functions as a reversible rectifier, in which an ac bias current induces a dc voltage. Besides the change in the sign of the output voltage (voltage polarity) could be governed by the applied magnetic field. Sputtering, electron beam lithography and ion etching techniques fabricate this versatile nanodevice. The samples are superconducting Nb films grown on arrays of nanometric Ni triangles. A magnetic field, applied on the nanostructured sample, sets up a lattice of vortices of magnetic flux quanta. The magnetic Ni triangles suppress the superconductivity and the vortices are pinned by the triangles. Increasing the magnetic field induces interstitial vortices.

When the system is driven with an external ac current a Lorentz force is pushing the vortices; they move in an array of asymmetric potentials (the triangles). This ratchet potential produces a net flow of vortices. The vortices on the triangles and the interstitial vortices feel a reversed ratchet potential, with different strength. The competition between these two potentials allows the tuning of the polarity of the output voltage.



Scanning Electron Microscope image of an array of Ni triangles. The side of the triangles is 500 nm. The position (circle) and motion (arrow) of the vortices (pinned vortices on the Ni triangles and interstitial vortices) are shown with circles and arrows.

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- Sergey Savel'ev (Frontier Research System, The Inst. of Physical and Chemical Research (RIKEN), Saitama, Japan).
- Franco Nori (Frontier Research System, The Inst. of Physical and Chemical Research (RIKEN), Saitama, Japan) / (Center for Theoretical Physics, Dept. of Physics, Univ. of Michigan, MI, USA).
- J. V. Anguita, R. García (Inst. de Microelectrónica de Madrid, Centro Nacional Mícroelectrónica, CSIC, Madrid, Spain).

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Science 302, 1188, 2003

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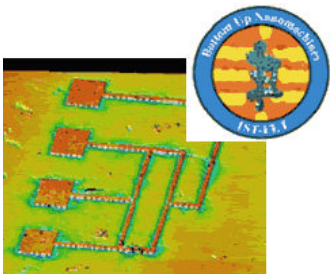

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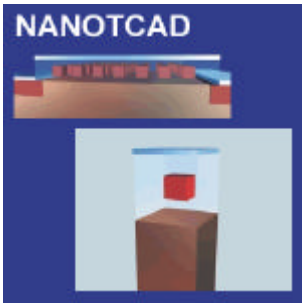

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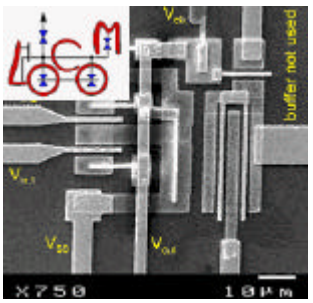

Latest Publications by PHANTOMS Members (1)

Physical Review B

Atomic-scale visualization and surface electronic structure of the hydrogenated diamond C(100)-(2×1):H surface Kirill Bobrov(1), Andrew Mayne(1), Geneviève Comtet(1,2), **Gérald Dujardin** (1,2), Lucette Hellner(1,2) and Alon Hoffman(3). (1)Lab. de Photophysique Moléculaire, Univ. Paris-Sud, Orsay Cedex, France. (2)Lab. pour l'Utilisation du Rayonnement Electromagnétique (LURE), Univ. Paris-Sud, Orsay Cedex, France. (3)Dept. of Chemistry and Solid State Inst., Technion Israel Inst. of Technology, Israel. Phys. Rev. B 68, 195416. 15 November 2003

Towards chemical identification in atomic-resolution noncontact AFM imaging with silicon tips A. S. Foster (Lab. of Physics, Helsinki Univ. of Technology, Finland), A. Y. Gal (Dept. of Physics and Astronomy, Univ. College London, London, UK), J. M. Airaksinen, O. H. Pakarinen, and Y. J. Lee (Lab. of Physics, Helsinki Univ. of Technology, Finland), J. D. Gale (Dept. of Chemistry, Imperial College London, London, UK), A. L. Shluger (Dept. of Physics and Astronomy, Univ. College London, London, UK), **R. M. Nieminen** (Lab. of Physics, Helsinki Univ. of Technology, Finland). Phys. Rev. B 68, 195420. 15 November 2003

Enhanced transmission of THz radiation through subwavelength holes J. Gómez Rivas, C. Schotsch, **P. Haring Bolivar**, and H. Kurz (Inst. für Halbleitertechnik, RWTH Aachen, Aachen, Germany). Phys. Rev. B 68, 201306(R). 15 November 2003

Electron energy loss spectroscopy as a probe of two-dimensional photonic crystals F. J. García de Abajo(1), A. Rivacoba(1), N. Zabala(1,2) and **P. M. Echenique**(1). (1)Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC), San Sebastián, Spain. (2)Dept. de Electricidad y Electrónica, Fac. de Ciencias, Bilbao, Spain. Phys. Rev. B 68, 205105. 15 November 2003

First-principles calculation of the electron inelastic mean free path in Be metal V. M. Silkin(1), E. V. Chulkov(1,2) and **P. M. Echenique**(1,2). (1)Donostia International Physics Center (DIPC) and Centro Mixto CSIC-UPV/EHU, San Sebastián/Donostia, Basque Country, Spain. (2)Dept. de Física de Materiales, Fac. de Ciencias Químicas, UPV/EHU, San Sebastián/Donostia, Basque Country, Spain. Phys. Rev. B 68, 205106. 15 November 2003

Calculated properties of nitrogen-vacancy complexes in beryllium- and magnesium-doped GaN C. D. Latham and R. Jones (School of Physics, Univ. of Exeter, Exeter, UK), S. Öberg (Dept. of Mathematics, Luleå Univ. of Technology, Luleå, Sweden), **R. M. Nieminen** (Lab. of Physics, Helsinki Univ. of Technology, Finland), P. R. Briddon (Physics Centre, School of Natural Science, Univ. of Newcastle upon Tyne, Newcastle, UK). Phys. Rev. B 68, 205209. 15 November 2003

Spin-polarized ballistic transport in diluted magnetic semiconductor quantum wire systems Kai Chang(1,2) and **F. M. Peeters**(1). (1)Dept. of Physics, Univ. of Antwerp (UIA), Antwerpen, Belgium. (2)NLSM, Inst. of Semiconductors, Chinese Academy of Sciences, Beijing, China. Phys. Rev. B 68, 205320. 15 November 2003

Limitation of the mobility of charge carriers in a nanoscaled heterogeneous system by dynamical Coulomb screening V. Kytin and Th. Dittrich (Hahn-Meitner-Inst., Berlin, Germany), **J. Bisquert** (Dept. de Ciències Experimentals, Univ. Jaume I, Castelló, Spain), E. A. Lebedev (Ioffe Physico-Technical Inst., St. Petersburg, Russia), F. Koch (Technische Univ. München, Physik Dept., Garching, Germany). Phys. Rev. B 68, 195308. 15 November 2003

Schottky barrier height at an organic/metal junction: A first-principles study of PTCDA/X (X = Al, Ag) contacts S. Picozzi (Ist. Nazionale di Fisica della Materia (INFM), Dipt. di Fisica, Univ. L'Aquila, L'Aquila, Italy), A. Pecchia, M. Gheorghe, **A. Di Carlo**, and P. Lugli (Ist. Nazionale di Fisica della Materia (INFM), Dipt. di Ingegneria Elettronica, Univ. Tor Vergata, Roma, Italy), B. Delley (Paul Scherrer Inst., Villigen PSI, Switzerland), M. Elstner (Dept. of Physics, Univ. of Paderborn, Germany). Phys. Rev. B 68, 195309. 15 November 2003

Simulating atomic force microscopy imaging of the ideal and defected TiO2 (110) surface A. S. Foster(1), O. H. Pakarinen(1), J. M. Airaksinen(1), J. D. Gale(2), and **R. M. Nieminen**(1). (1)Lab. of Physics, Helsinki Univ. of Technology, Helsinki, Finland. (2)Dept. of Chemistry, Imperial College London, UK. Phys. Rev. B 68, 195410. 15 November 2003

a- and b-tricalcium phosphate: A density functional study Xilin Yin and M. J. Stott (Dept. of Physics, Queen's Univ., Kingston, Ontario, Canada), A. Rubio (**Dpto. Física de Materiales, Fac. de Químicas, Univ. del País Vasco UPV/EHU, Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC), San Sebastián/Donostia, España**). Phys. Rev. B 68, 205205. 15 November 2003

Four-electron quantum dot in a magnetic field M. B. Tavernier(1), E. Anisimovas(1), **F. M. Peeters**(1), B. Szafran(1,2), J. Adamowski(2), and S. Bednarek(2) (1)Dept. Natuurkunde, Univ. Antwerpen (Campus Drie Eiken), Antwerpen, Belgium. (2)Fac. of Physics and Nuclear Techniques, AGH Univ. of Science and Technology, Kraków, Poland. Phys. Rev. B 68, 205305. 15 November 2003

Stability and transition between vortex configurations in square mesoscopic samples with antidots G. R. Berdiyorov, B. J. Baelus, M. V. Milo evi , and **F. M. Peeters** (Dept. Natuurkunde, Univ. Antwerpen (Campus Drie Eiken), Antwerpen, Belgium. Phys. Rev. B 68, 174521. 01 November 2003

Ab initio determination of the ground-state properties of Ca2MgSi2O7 åkermanite Razvan Caracas and **Xavier Gonze** (Univ. Catholique de Louvain, Unité de Physico-Chimie et de Physique de Matériaux, Louvain-la-Neuve, Belgium). Phys. Rev. B 68, 184102. 01 November 2003

Magnetic origin of enhanced top exchange biasing in Py/IrMn/Py multilayers G. Malinowski, M. Hehn, S. Robert, O. Lenoble, and **A. Schuhl** (Lab. de Physique des Matériaux, UMR CNRS 7556, Vandoeuvre lès Nancy Cedex, France), P. Panissod (IPCMS, Groupe d'étude des matériaux métalliques, UMR CNRS 7504, Strasbourg, France). Phys. Rev. B 68, 184404. 01 November 2003

Quantum pumping: Coherent rings versus open conductors M. Moskalets(1) and **M. Büttiker**(2). (1)Dept. of Metal and Semiconductor Physics, National Technical Univ. "Kharkov Polytechnical Inst.," Kharkov, Ukraine. (2)Dept. de Physique Théorique, Univ. de Genève, Genève 4, Switzerland. Phys. Rev. B 68, 161311(R). 15 October 2003

Ordering tendencies in octahedral MgO-ZnO alloys Mahdi Sanati(1), Gus L. W. Hart(2), and **Alex Zunger**(1). (1)National Renewable Energy Lab., Golden, Colorado, USA. (2)Dept. of Physics & Astronomy, Northern Arizona Univ., Arizona, USA. Phys. Rev. B 68, 155210. 15 October 2003

Latest Publications by PHANTOMS Members (2)

Physical Review B

Resonance Kondo tunneling through a double quantum dot at finite bias M. N. Kiselev(1), K. Kikoin(2), and **L. W. Molenkamp**(3). (1)Inst. für Theoretische Physik, Univ. Würzburg, Würzburg, Germany. (2)Ben-Gurion Univ. of the Negev, Beer-Sheva, Israel. (3)Physikalisches Inst. (EP 3), Univ. Würzburg, Würzburg, Germany. Phys. Rev. B 68, 155323. 15 October, 2003

Predicting interband transition energies for InAs/GaSb superlattices using the empirical pseudopotential method Rita Magri (Ist. Nazionale per la Fisica della Materia, S3, and Dip. di Fisica Univ. di Modena e Reggio Emilia, Modena, Italy), **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 155329. 15 October, 2003

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Adjusting the coherent transport in finite periodic superlattices C. Pacher and **E. Gornik** (Inst. für Festkörperelektronik und Mikrostrukturzentrum, Technische Univ. Wien, Wien, Austria). Phys. Rev. B 68, 155319. 15 October 2003

Superstructures and coincidences of a thin oxide film on a metallic substrate: A STM study T. Maroutian(1), S. Degen(2), C. Becker(2), K. Wandelt(2), and **R. Berndt**(1). (1)Inst. für Experimentelle und Angewandte Physik, Christian-Albrechts-Univ. zu Kiel, Kiel, Germany. (2)Inst. für Physikalische und Theoretische Chemie, Univ. Bonn, Bonn, Germany. Phys. Rev. B 68, 155414. 15 October 2003

Relaxation of high-energy quasiparticle distributions: Electron-electron scattering in a two-dimensional electron gas R. N. Gurzhi, A. I. Kopeliovich, A. N. Kalinenko, and A. V. Yanovsky (B. Verkin Inst. for Low Temperature Physics & Engineering, National Academy of Sciences of Ukraine, Kharkov, Ukraine), E. N. Bogachek and Uzi Landman (School of Physics, Georgia Inst. of Technology, Atlanta, Georgia, USA), H. Buhmann and **L. W. Molenkamp** (Physikalisches Inst. der Univ. Würzburg, Würzburg, Germany). Phys. Rev. B 68, 165318. 15 October 2003

Infrared investigation of the low-temperature structural and magnetic transitions in the spin-ladder candidate (DT-TTF)$_2$Au(mnt)$_2$ R. Weso owski and J. T. Haraldsen (Dept. of Physics and Astronomy, Univ. of Tennessee, Knoxville, Tennessee, USA), J. L. Musfeldt (Dept. of Chemistry, Univ. of Tennessee, Knoxville, Tennessee, USA), T. Barnes (Dept. of Physics and Astronomy, Univ. of Tennessee, Knoxville, Tennessee, USA / Physics Division, Oak Ridge National Lab., Oak Ridge, Tennessee, USA), M. Mas-Torrent and C. Rovira (**Inst. de Ciéncia dels Materials de Barcelona, Campus de la U. A. B., Bellaterra, Spain**), R. T. Henriques and M. Almeida (Dept. de Quimica, ITN, Sacaven Codex, Portugal). Phys. Rev. B 68, 134405. 01 October 2003

Intersubband plasmons in quasi-one-dimensional electron systems on a liquid helium surface Marcos R. S. Tavares (Fac. de Tecnologia da Baixada Santista, CEETPS, São Paulo, Brazil), G.-Q. Hai (Inst. de Física de São Carlos, Unv. de São Paulo, São Paulo, Brazil), **F. M. Peeters** (Dept. of Physics, Univ. of Antwerp (UIA), Antwerpen, Belgium), Nelson Studart (Dept. de Física, Univ. Federal de São Carlos, São Paulo, Brazil). Phys. Rev. B 68, 140504(R). 01 October 2003

First-principles investigation of phonon softenings and lattice instabilities in the shape-memory system Ni2MnGa A. T. Zayak and P. Entel (Inst. of Physics, Gerhard-Mercator Univ., Duisburg, Germany), J. Enkovaara, A. Ayuela, and **R. M. Nieminen** (Lab. of Physics, Helsinki Univ. of Technology, Espoo, Finland). Phys. Rev. B 68, 132402 (2003). 1 October 2003

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Conductance switching in a molecular device: The role of side groups and intermolecular interactions Jeremy Taylor, Mads Brandbyge, and **Kurt Stokbro** (Mikroelektronik Centret (MIC), Technical Univ. of Denmark (DTU), Lyngby, Denmark). Phys. Rev. B 68, 121101(R) (2003). 15 September 2003

Dilute nonisovalent (II-VI)-(III-V) semiconductor alloys: Monodoping, codoping, and cluster doping in ZnSe-GaAs L. G. Wang and **Alex Zunger** (National Renewable Energy Lab., Colorado, USA). Phys. Rev. B 68, 125211 (2003). 15 September 2003

Correlation between overgrowth morphology and optical properties of single self-assembled InP quantum dots M. K.-J. Johansson, U. Håkanson, M. Holm, J. Persson, T. Sass, and J. Johansson (Solid State Physics/Nanometer Consortium, Lund Univ., Lund, Sweden), C. Pryor (Optical Science and Technology Center, Univ. of Iowa, Iowa City, Iowa, USA), L. Montelius, W. Seifert, **L. Samuelson**, and M.-E. Pistol (Solid State Physics/Nanometer Consortium, Lund Univ., Lund, Sweden). Phys. Rev. B 68, 125303 (2003). 15 September 2003

Characterization of GaN quantum discs embedded in AlxGa1-xN nanocolumns grown by molecular beam epitaxy J. Risti, E. Calleja, M. A. Sánchez-García, and J. M. Ulloa (**ISOM and Dept. Ingeniería Electrónica, ETSI Telecomunicación, Univ. Politécnica de Madrid, Madrid, Spain**), J. Sánchez-Páramo and J. M. Calleja (Dept. Física de Materiales, Univ. Autónoma de Madrid, Madrid, Spain), U. Jahn, A. Trampert, and K. H. Ploog (Paul-Drude-Inst. Für Festkörperelektronik, Berlin, Germany). Phys. Rev. B 68, 125305 (2003). 15 September 2003

Interaction between a superconducting vortex and an out-of-plane magnetized ferromagnetic disk: Influence of the magnet geometry M. V. Miloevi and **F. M. Peeters** (Dept. Natuurkunde, Univ. Antwerpen (UIA), Antwerpen, Belgium). Phys. Rev. B 68, 094510 (2003). 1 September 2003

Pair breaking by chain oxygen disorder in light-ion irradiated YBa2Cu3Ox thin films D. Arias(1)Z. Sefrioui(1)G. D. Loos(1)**F. Agullo-Rueda**(2)J. Garcia-Barriocanal(1)C. Leon(1)and J. Santamaria(1). (1)GFMC, Dept. de Fisica Aplicada III, Facultad de Fisica, UCM, Madrid, Spain. (2)Inst. de Ciencia de Materiales de Madrid (ICMM-CSIC), Cantoblanco, Spain. Phys. Rev. B 68, 094515 (2003). 1 September 2003

s-d coupling in zinc-blende semiconductors Clas Persson and **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 073205 (2003).15 August 2003

Latest Publications by PHANTOMS Members (3)

Physical Review B

Compositional and size-dependent spectroscopic shifts in charged self-assembled InxGa1-xAs/GaAs quantum dots Gabriel Bester and **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 073309 (2003). 15 August 2003

n-type doping and passivation of CuInSe2 and CuGaSe2 by hydrogen Çetin Klç and **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 075201 (2003). 15 August 2003

Ferromagnetism in Mn-doped GaAs due to substitutional-interstitial complexes Priya Mahadevan and **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 075202 (2003). 15 August 2003

Hidden quantum pump effects in quantum coherent rings M. Moskalets(1) and **M. Büttiker**(2). (1)Dept. of Metal and Semiconductor Physics, National Technical Univ. "Kharkov Polytechnical Inst.," Kharkov, Ukraine. (2)Dépt. de Physique Théorique, Univ. de Genève, Genève, Switzerland. Phys. Rev. B 68, 075303 (2003). 15 August 2003

Role of energy correlations on Coulomb suppression of shot noise in ballistic conductors contacted to degenerate reservoirs T. González, J. Mateos, and **D. Pardo** (Dept. de Física Aplicada, Univ. de Salamanca, Salamanca, Spain), G. Gomila (**Dept. d'Electrònica and CBEN, Univ. de Barcelona, Barcelona, Spain**), I. R. Cantalapiedra (Dept. de Física Aplicada, Univ. Politècnica de Catalunya, Barcelona, Spain), L. Reggiani (**INFM-National Nanotechnology Lab. and Dipt. di Ingegneria dell'Innovazione, Univ. di Lecce, Lecce, Italy**). Phys. Rev. B 68, 075309 (2003). 15 August 2003

Hot-electron lifetimes in metals: A combined ab initio calculation and ballistic electron emission spectroscopy analysis Florian Ladstädter(1), Pilar F. de Pablos(2), Ulrich Hohenester(1), Peter Puschnig(1), Claudia Ambrosch-Draxl(1), Pedro L. de Andrés(3), Francisco J. García-Vidal(2), and **Fernando Flores**(2). (1)Inst. für Theoretische Physik, Karl-Franzens-Univ. Graz, Graz, Austria. (2)Dept. de Física Teórica de la Materia Condensada, U. Autónoma de Madrid, Madrid, Spain. (3)Inst. de Ciencia de Materiales (CSIC), Madrid, Spain. Phys. Rev. B 68, 085107 (2003). 15 August 2003

First-principles simulations of the stretching and final breaking of Al nanowires: Mechanical properties and electrical conductance Pavel Jelínek(1,2)Rubén Pérez(1)José Ortega(1)and **Fernando Flores**(1). (1)Dept. de Física Teórica de la Materia Condensada, Univ. Autónoma de Madrid, Spain. (2)Inst. of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic. Phys. Rev. B 68, 085403 (2003). 15 August 2003

Origin of complex exchange anisotropy in Fe/MnF2 bilayers I. N. Krivorotov(1), C. Leighton(2), J. Nogués(3), **Ivan K. Schuller**(4), and E. Dan Dahlberg(1). (1)Dept. of Physics, Univ. of Minnesota, Minneapolis, Minnesota, USA. (2)Dept. of Chemical Engineering and Materials Science, Univ. of Minnesota, Washington Avenue SE, Minneapolis, Minnesota, USA. (3)Inst. Catalana de Recerca i Estudis Avançats (ICREA) and Dept. de Física, Univ. Autònoma de Barcelona, Bellaterra, Spain. (4)Dept. of Physics, Univ. of California-San Diego, La Jolla, California, USA. Phys. Rev. B 68, 054430 (2003). 1 August 2003

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Analysis of structure and vibrational dynamics of the BeTe(001) surface using x-ray diffraction, Raman spectroscopy, and density functional theory C. Kumpf, A. Müller, W. Weigand, and E. Umbach (Lehrstuhl für Experimentelle Physik II, Univ. Würzburg, Würzburg, Germany), J. Wagner, V. Wagner, S. Gundel, L. Hansen, and J. Geurts (**Lehrstuhl für Experimentelle Physik III, Univ. Würzburg, Würzburg, Germany**), O. Bunk (Materials Research Dept., Risø National Lab., Roskilde, Denmark), J. H. Zeysing, F. Wu, and R. L. Johnson (Inst. für Experimentalphysik, Univ. Hamburg, Hamburg, Germany). Phys. Rev. B 68, 035339 (2003). 15 July 2003

Dynamic response of a strongly perturbed electron gas R. Díez Muiño(1), A. Arnau(2), A. Salin(1,3), and **P. M. Echenique**(1,2). (1)Donostia International Physics Center (DIPC), San Sebastián, Spain. (2)Dept. de Física de Materiales, Facultad de Químicas UPV/EHU, and Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain. (3)Lab. de Physico-Chimie Moléculaire, UMR 5803 CNRS-Univ. de Bordeaux I, Talence Cedex, France. Phys. Rev. B 68, 041102(R) (2003). 15 July 2003

Preparation, structure, and electronic properties of Fe3O4 films on the Fe(110)/Mo(110)/Al2O3(110) substrate M. Fonin(1), Yu. S. Dedkov(1), J. Mayer(2), U. Rüdiger(1,3), and **G. Güntherodt**(1). (1)II. Physikalisches Inst., Rheinisch-Westfälische Technische Hochschule Aachen, Aachen, Germany. (2)Gemeinschaftslabor für Elektronenmikroskopie, Rheinisch-Westfälische Technische Hochschule Aachen, Aachen, Germany. (3)Fachbereich Physik, Univ. Konstanz, Konstanz, Germany. Phys. Rev. B 68, 045414 (2003). 15 July 2003

Orientation and constraints of endohedral lanthanum in La@C82 molecules adsorbed on Cu(111) C. Ton-That(1), A. G. Shard(2), S. Egger(1), V. R. Dhanak(3), A. Taninaka(4), H. Shinohara(4), and **M. E. Welland**(1). (1)Nanoscience Centre, Univ. of Cambridge, Cambridge, UK. (2)Dept. of Engineering Materials, Univ. of Sheffield, Sheffield, UK. (3)SRS Daresbury Lab. and Physics Dept., Univ. of Liverpool, UK). (4)Dept. of Chemistry, Nagoya Univ., Nagoya, Japan. Phys. Rev. B 68, 045424 (2003). 15 July 2003

Ab initio calculations of the lattice dynamics of boron nitride nanotubes Ludger Wirtz and **Angel Rubio** (Dept. of Material Physics, Univ. of the Basque Country, Centro Mixto CSIC-UPV, and Donostia International Physics Center, Donostia-San Sebastián, Spain), Raul Arenal de la Concha and Annick Loiseau (LEM, ONERA-CNRS, Châtillon Cedex, France). Phys. Rev. B 68, 045425 (2003). 15 July 2003

Deep nitrogen-induced valence- and conduction-band states in GaAs1-xNx Clas Persson and **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado, USA). Phys. Rev. B 68, 035212 (2003). 1 july 2003

Latest Publications by PHANTOMS Members (4)

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Latest Publications by PHANTOMS Members (8)

Nanotechnology

Parallel information and computation with restitution for noise-tolerant nanoscale logic networks Akram S Sadek, Konstantin Nikolic and **Michael Forshaw** (Image Processing Group, Dept. of Physics and Astronomy, Univ. College London, London, UK). Nanotechnology 15 (January 2004) 192-210

Direct writing of ZrO2 on a sub-10 nm scale using an electron beam K R V Subramanian(1), M S M Saifullah(1,3), E Tapley(2), Dae-Joon Kang(1), **M E Welland**(1) and M Butler(2). (1) The Nanoscience Centre, Interdisciplinary Research Collaboration in Nanotechnology, Univ. of Cambridge, Cambridge, UK. (2)Leica Microsystems Lithography Limited, Cambridge, UK. Nanotechnology 15 (January 2004) 158-162

Combinatorial chips for optimizing the growth and integration of carbon nanofibre based devices Alan M Cassell, Qi Ye, Brett A Cruden, Jun Li, Philippe C Sarrazin, Hou Tee Ng, Jie Han and **M Meyyappan** (Center For Nanotechnology, NASA Ames Research Center, CA, USA). Nanotechnology 15 (January 2004) 9-15

Metal patterned highly oriented pyrolytic graphite as a template for direct polymer molding Y Gimeno(1), A Hernández Creus(1), S González(1), O Azzaroni(2), P L Schilardi(2) and **R C Salvarezza**(1,2). (1)Dept. de Química Física, Univ. de la Laguna, Tenerife, Spain. (2) Inst. de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), Univ. Nacional de La Plata-CONICET, La Plata, Argentina. Nanotechnology 15 (January 2004) 82-85

Ultrasensitive label-free DNA analysis using an electronic chip based on carbon nanotube nanoelectrode arrays Jessica Koehne, Hua Chen(1), Jun Li, Alan M Cassell(1), Qi Ye(1), Hou Tee Ng(1), Jie Han(1) and **M Meyyappan**. NASA Ames Research Center, Moffett Field, CA 94035, USA. (1)ELORET Corporation, Sunnyvale, CA 94087, USA. Nanotechnology 14 (December 2003) 1239-1245

Fabrication of individually seeded nanowire arrays by vapour-liquid-solid growth T Mårtensson, M Borgström, W Seifert, B J Ohlsson(1) and **L Samuelson**. Solid State Physics/The Nanometer Consortium, Lund University, PO Box 118, SE-221 00 Lund, Sweden. (1)Now at: QuMat Technologies AB, Magle Stora Kyrkogata 8, SE-223 50 Lund, Sweden Nanotechnology 14 (December 2003) 1255-1258

Effect of high temperature annealing on the charge trapping characteristics of silicon nanocrystals embedded within SiO2 V Ioannou-Sougleridis(1), **A G Nassiopoulou**(1) and A Travlos(2). (1)IMEL/NCSR Demokritos, Aghia Paraskevi, Athens, Greece. (2)IMS/NCSR Demokritos, Aghia Paraskevi, Athens, Greece. Nanotechnology 14 (November 2003) 1174-1179

Towards in-plane metathesis polymerization at self-assembled monolayers of norbornene adsorbates on gold surfaces Xue-Mei Li, **Jurriaan Huskens** and David N Reinhoudt (Lab. of Supramolecular Chemistry and Technology, MESA+ Research Inst., Univ. of Twente, Enschede, The Netherlands). Nanotechnology 14 (October 2003) 1064-1070

Atomistic modelling of nanostructures via the Bozzolo-Ferrante-Smith quantum approximate method Guillermo Bozzolo(1,2), Jorge E Garcés(3), Ronald D Noebe(2) and Daniel Farías(4). (1)OAI, Cedar Point Road, Cleveland, USA. (2)NASA Glenn Research Center, Cleveland, USA. (3)Centro Atómico Bariloche, Bariloche, Argentina. (4)**Dept. de Física de la Materia Condensada, Univ. Autónoma de Madrid, Madrid, Spain**. Nanotechnology 14 (September 2003) 939-945.

Journal of Physical Chemistry B

Electrodesorption Potentials of Self-Assembled Alkanethiolate Monolayers on Copper Electrodes. An Experimental and Theoretical Study O. Azzaroni, M. E. Vela, M. Fonticelli, G. Benítez, P. Carro, B. Blum, and **R. C. Salvarezza**. J. Phys. Chem. B; 2003; 107(48) pp 13446 - 13454. 04 December 2003

Comment on "Diffusion Impedance and Space Charge Capacitance in the Nanoporous Dye-Sensitized Electrochemical Solar Cell" and "Electronic Transport in Dye-Sensitized Nanoporous TiO2 Solar Cells-Comparison of Electrolyte and Solid-State Devices" **Juan Bisquert**. J. Phys. Chem. B; 2003; 107(48) pp 13541 - 13543. 04 December 2003

Reversibly Altering Electronic Conduction through a Single Molecule by a Chemical Binding Event Bala Sundari T. Kasibhatla, André P. Labonté, Ferdows Zahid, **Ronald G. Reifenberger**, Supriyo Datta, and Clifford P. Kubiak. J. Phys. Chem. B; 2003; 107(45) pp 12378 - 12382. 13 November 2003

Flatband Potential of F:SnO2 in a TiO2 Dye-Sensitized Solar Cell: An Interference Reflection Study M. Turrión, **J. Bisquert**, and P. Salvador. J. Phys. Chem. B; 2003; 107(35) pp 9397 - 9403. 4 September 2003

Self-Assembled Gold Nanoparticle/Alkanedithiol Films: Preparation, Electron Microscopy, XPS-Analysis, Charge Transport, and Vapor-Sensing Properties Yvonne Joseph, Isabelle Besnard, Miriam Rosenberger, Berit Guse, Heinz-Georg Nothofer, **Jurina M. Wessels**, Ute Wild, Axel Knop-Gericke, Dangsheng Su, Robert Schlögl, Akio Yasuda, and Tobias Vossmeyer. J. Phys. Chem. B; 2003; 107(30) pp 7406 - 7413. 31 July 2003

Nature

Single-electron transistor of a single organic molecule with access to several redox states Sergey Kubatkin(1), Andrey Danilov(1), Mattias Hjort(2), **Jérôme Cornil**(2,3), Jean-Luc Brédas(2,3,*), Nicolai Stuhr-Hansen(4), Per Hedegård(4) and **Thomas Bjørnholm**(4). (1)**Dept. of Microtechnology and Nanoscience/MC2, Univ. of Technology, Chalmers, Göteborg, Sweden** . (2)Dept. of Chemistry, The Univ. of Arizona, Tucson, Arizona, USA. (3)Lab. for Chemistry of Novel Materials, Center for Research in Molecular Electronics and Photonics, Univ. of Mons-Hainaut, Mons, Belgium. (4)Nano-Science Center (Dept. of Chemistry and Niels Bohr Insti.), Univ. of Copenhagen, Copenhagen, Denmark. (*)Present address: School of Chemistry and Biochemistry, Georgia Inst. of Technology, Atlanta, Georgia, USA. Nature 425, 698 - 701 (16 October 2003); doi:10.1038/nature02010

Latest Publications by PHANTOMS Members (9)

Journal of Chemical Physics

Velocity redistribution of excited atoms by radiative excitation transfer. II. Theory of radiation trapping in collimated beams N. N. Bezuglov (St. Petersburg State Univ., Fock Inst. of Physics, St. Petersburg, Russia), A. Ekers, O. Kaufmann, and K. Bergmann (Univ. of Kaiserslautern, Dept. of Physics, Kaiserslautern, Germany), F. Fuso and M. Allegrini (**INFM, Dipt. di Fisica Enrico Fermi, Univ. di Pisa, Pisa, Italy**). The Journal of Chemical Physics -- October 8, 2003 -- Volume 119, Issue 14, pp. 7094-7110

Modeling the bacterial photosynthetic reaction center. VII. Full simulation of the intervalence hole-transfer absorption spectrum of the special-pair radical cation Jeffrey R. Reimers (School of Chemistry, The Univ. of Sydney, Australia), **Noel S. Hush** (School of Molecular and Microbial Biosciences and the School of Chemistry, The Univ. of Sydney, New South Wales, Australia). The Journal of Chemical Physics -- August 8, 2003 -- Volume 119, Issue 6, pp. 3262-3277

Modeling the bacterial photosynthetic reaction center. VI. Use of density-functional theory to determine the nature of the vibronic coupling between the four lowest-energy electronic states of the special-pair radical cation Jeffrey R. Reimers and Warwick A. Shapley (School of Chemistry, The Univ. of Sydney, Australia), Alistair P. Rendell (Dept. of Computer Science, Australian National Univ., Australia), **Noel S. Hush** (School of Chemistry and School of Molecular and Microbial Biosciences, The Univ. of Sydney, Australia). The Journal of Chemical Physics -- August 8, 2003 -- Volume 119, Issue 6, pp. 3249-3261

Modelling the bacterial photosynthetic reaction center. V. Assignment of the electronic transition observed at 2200 cm-1 in the special-pair radical-cation as a second-highest occupied molecular orbital to highest occupied molecular orbital transition Jeffrey R. Reimers and Warwick A. Shapley (School of Chemistry, The Univ. of Sydney, Australia), **Noel S. Hush** (School of Chemistry and School of Molecular and Microbial Biosciences, The Univ. of Sydney, Australia). The Journal of Chemical Physics -- August 8, 2003 -- Volume 119, Issue 6, pp. 3240-3248

Science

A Superconducting Reversible Rectifier That Controls the Motion of Magnetic Flux Quanta J. E. Villegas(1), Sergey Savel'ev(2), Franco Nori(2,3), E. M. Gonzalez(1), J. V. Anguita(4), **R. García**(4), J. L. Vicent(1). (1)Dept. de Física de Materiales, Fac. Ciencias Físicas, Univ. Complutense, Madrid, Spain. (2)Frontier Research System, The Inst. of Physical and Chemical Research (RIKEN), Saitama, Japan. (3)Center for Theoretical Physics, Dept. of Physics, Univ. of Michigan, MI, USA. (4)Inst. de Microelectrónica de Madrid, Centro Nacional Mícroelectrónica, CSIC, Madrid, Spain. Science, Volume 302, Number 5648, Issue of 14 Nov 2003, pp. 1188-1191.

Latest Publications by PHANTOMS Members (10)

J. Vacuum Science & Technology B: Microelectronics & Nanometer Structures

Electric field effects in single semiconductor quantum dots observed by scanning tunneling luminescence U. Håkanson, H. Håkanson, M. K.-J. Johansson, **L. Samuelson**, and M.-E. Pistol (Solid State Physics/The Nanometer Consortium, Lund Univ., Lund, Sweden). Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures -- November 2003 -- Volume 21, Issue 6, pp. 2344-2347

High aspect ratio nano-oxidation of silicon with noncontact atomic force microscopy N. Clement, **D. Tonneau**, B. Gely, H. Dallaporta, and V. Safarov (GPEC, Fac. des Sciences de Luminy, Marseille Cedex 9, France), J. Gautier (CEA-DRT LETI-DTS Grenoble, Grenoble Cedex, France). Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures -- November 2003 -- Volume 21, Issue 6, pp. 2348-2351

Emission characteristics of ultrathin layer solid-state emitters, temperature, and thickness dependence H. Nakane, J. P. Dupin, and **Vu Thien Binh** (Lab. d'Emission Electronique DPM-CNRS, Univ. Claude Bernard Lyon 1, Villeurbanne, France). Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures -- July 2003 -- Volume 21, Issue 4, pp. 1616-1617

Theory of optical properties of 6.1 Å III-V superlattices: The role of the interfaces Rita Magri (Ist. Nazionale per la Fisica della Materia, S3, and Dipt. di Fisica Univ. di Modena e Reggio Emilia, Modena, Italy), **Alex Zunger** (National Renewable Energy Lab., Golden, Colorado). Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures -- July 2003 -- Volume 21, Issue 4, pp. 1896-1902

Nanoletters

Multiple Length Scale Patterning of Single-Molecule Magnets Massimiliano Cavallini, Fabio Biscarini, Jordi Gomez-Segura, Daniel Ruiz, and **Jaume Veciana**. Nano Lett.; 2003; 3(11) pp 1527 - 1530. 12 November 2003

Band Gap Photobleaching in Isolated Single-Walled Carbon Nanotubes Michael S. Arnold, Jay E. Sharping, Samuel I. Stupp, Prem Kumar, and **Mark C. Hersam**. Nano Lett.; 2003; 3(11) pp 1549 - 1554. 12 November 2003

Sub-10 nm Electron Beam Nanolithography Using Spin-Coatable TiO2 Resists M. S. M. Saifullah, K. R. V. Subramanian, E. Tapley, Dae-Joon Kang, **M. E. Welland**, and M. Butler. Nano Lett.; 2003; 3(11) pp 1587 - 1591. 12 November 2003

Selective Positioning and Density Control of Nanotubes within a Polymer Thin Film Emer Lahiff, Chang Y. Ryu, Seamus Curran, Andrew I. Minett, **Werner J. Blau**, and Pulickel M. Ajayan. Nano Lett.; 2003; 3(10) pp 1333 - 1337. 08 October 2003

Adlayers and Low-Dimensional Assemblies of a TTF Derivative at a Liquid-Solid Interface Mohamed M. S. Abdel-Mottaleb, Elba Gomar-Nadal, Steven De Feyter, Magdalena Zdanowska, **Jaume Veciana**, Concepció Rovira, David B. Amabilino, and Frans C. De Schryver. Nano Lett.; 2003; 3(10) pp 1375 - 1378. October 2003

Catalytic Microcontact Printing without Ink Xue-Mei Li, Mária Péter, **Jurriaan Huskens**, and David N. Reinhoudt **.** Nano Lett.; 2003; 3(10) pp 1449 - 1453. October 2003

Helium Detection via Field Ionization from Carbon Nanotubes David J. Riley, Mark Mann, Donald A. MacLaren, Paul C. Dastoor, William Allison, Kenneth B. K. Teo, Gehan A. J. Amaratunga, and **William Milne**. Nano Lett.; 2003; 3(10) pp 1455 - 1458. October 2003

Prediction of a Shape-Induced Enhancement in the Hole Relaxation in Nanocrystals Marco Califano, Gabriel Bester, and **Alex Zunger** . Nano Lett.; 2003; 3(9) pp 1197 - 1202. September 2003

Stretching and Transporting DNA Molecules Using Motor Proteins Stefan Diez, Cordula Reuther, Cerasela Dinu, Ralf Seidel, Michael Mertig, **Wolfgang Pompe**, and Jonathon Howard. Nano Lett.; 2003; 3(9) pp 1251 - 1254. September 2003

Nanostructuring Conjugated Materials by Lithographically Controlled Wetting Massimiliano Cavallini and Fabio Biscarini. Nano Lett.; 2003; 3(9) pp 1269 - 1271. September 2003

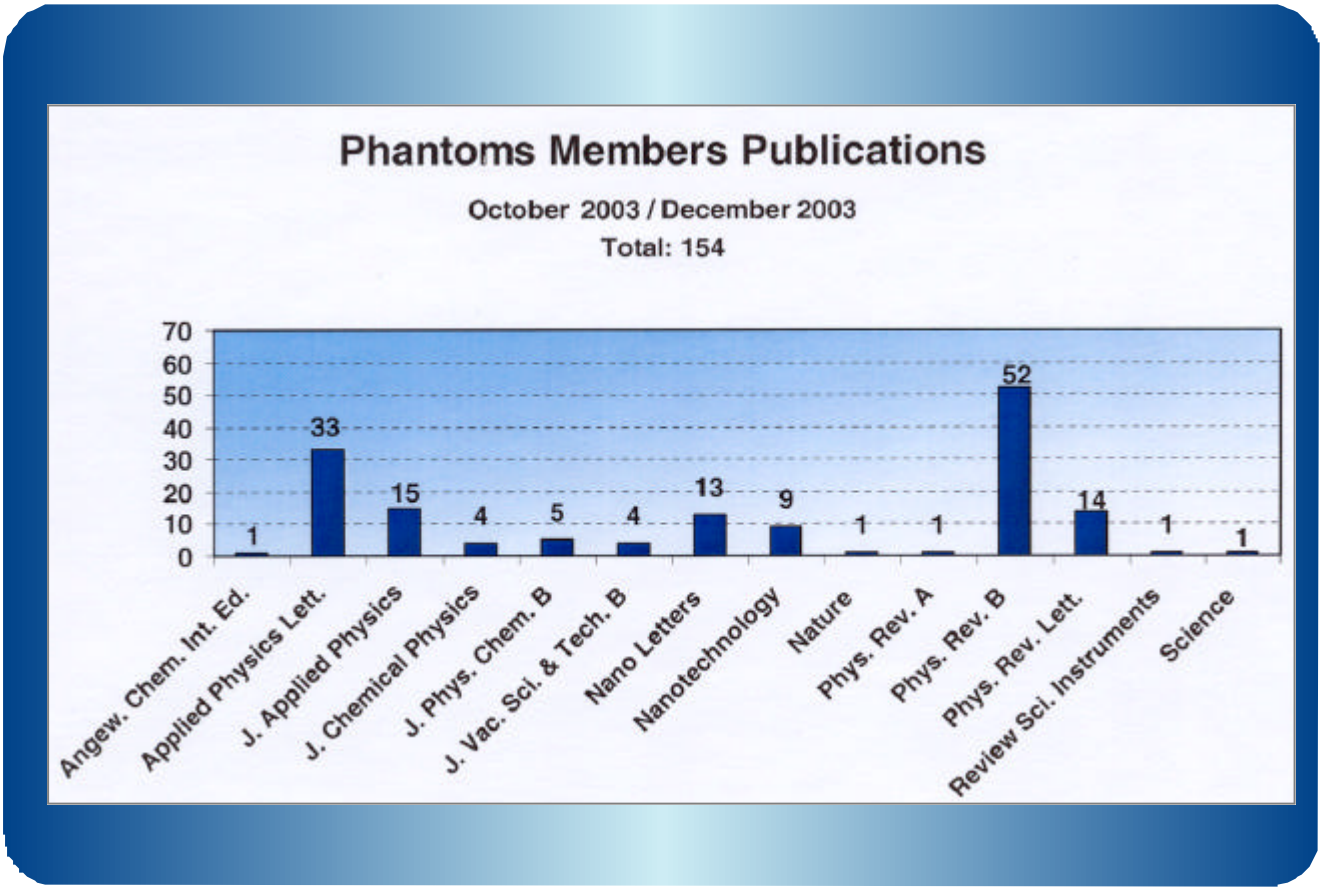
Optically Active Organic Microrings F. Balzer, J. Beermann, S. I. Bozhevolnyi, A. C. Simonsen, and **H.-G. Rubahn**. Nano Lett.; 2003; 3(9) pp 1311 - 1314. September 2003

Rectifying Behavior of Electrically Aligned ZnO Nanorods Oliver Harnack, Claudia Pacholski, Horst Weller, Akio Yasuda, and **Jurina M. Wessels**. Nano Lett.; 2003; 3(8) pp 1097 - 1101. August 2003

Schottky Barriers and Coulomb Blockade in Self-Assembled Carbon Nanotube FETs L. Marty, V. Bouchiat, C. Naud, M. Chaumont, T. Fournier, and **A. M. Bonnot**. Nano Lett.; 2003; 3(8) pp 1115 - 1118. August 2003

Angewandte Chemie International Edition

Cover Picture: Regulatory Strategies in the Complexation and Release of a Noncovalent Guest Trimer by a Self-Assembled Molecular Cage Jessica M. C. A. Kerckhoffs, Dr.(1), Fijs W. B. van Leeuwen(1), Anthony L. Spek, Prof. (2), Huub Kooijman, Dr.(2), Mercedes Crego-Calama, Dr.(1), **David N. Reinhoudt, Prof.**(1). (1)Lab. of Supramolecular Chemistry and Technology, MESA+ Research Inst., Univ. of Twente, Enschede, The Netherlands. (2)Dept. of Crystal and Structural Chemistry, Bijvoet Center for Biomolecular Research, Utrecht Univ., Utrecht, The Netherlands. Angewandte Chemie International Edition, Volume 42, Issue 46 , Pages 5653 - 5653. 01 December 2003



ADVERTISEMENTS

13th NID Workshop to be held in Athens (Greece), 4-6 February 2003

http://www.phantomsnet.com/nidconference7/homepage.php

The 13th NID Workshop will be organised in collaboration with the Institute of Microelectronics, NCSR Demokritos (Greece) and take place at the National Center for Scientific Research "Demokritos" located on the foot of Mount Hemittos at the outskirts of Aghia Paraskevi, a suburb of Athens, and about 12km to the north from downtown Athens.

IMEL, one of the eight Institutes of NCSR "Demokritos", specializing in silicon microelectronics, started its activitities in 1985. The expertise in VLSI design, CMOS processing, IC prototyping and special device fabrication developed over the years of its operation, supplemented by state-of-the-art facilities, make it unique in its field in the country.

The 13th NID workshop will gather participants in the projects funded within the NID pro-active initiative. Presentations from the EU projects and invited talks from experts outside the NID initiative will take place during the workshop and be focused on the application of a broad range of nano-scale technologies to information processing and on the perspectives for replacing mainstream approaches, such as CMOS, when they will reach the expected physical limits for miniaturisation.

The 13th NID workshop will be the last large event organised by the current PHANTOMS network. The Organising Commitee will revitalise the Working Groups by having them contribute to selected roadmaps to be discussed at the workshop.

NID **W**orking **G**roups are open for those colleagues interested.
Contact the Working Group coordinator to participate.
- **WG Mono-Molecular Electronics** (Christian Joachim - joachim@cemes.fr / Gerhard Meyer - gme@zurich.ibm.com)
- **WG Theory** (Jim Greer - jgreer@nmrc.ucc.ie)
- **WG Alternative Electronics** (Jean Nöel Patillon - patillon@crm.mot.com / Arianna Filoramo - filoramo@drecam.saclay.cea.fr)

The mission of the working groups is to enhance the research between the NID projects in particular to:

- Exchange information of current work
- Enhance the collaboration in the projects and promote new ones
- Solve particular technological problems
- Looking for areas of common ground between different technologies
- Give contributions to the roadmap / PHANTOMS Reports

Invited Speakers:

Prof. Efthymios Kaxiras
Harvard University (USA)
Prof. Konstantin K. Likharev
Stony Brook University (USA)

Greek Workshop:
Wednesday 4th of February 2004
A joint "Greek / PHANTOMS" Nanoworkshop (open to all participants) will be held in order to provide a research overview on Nanotechnology currently performed in this country.

Organising Committee:

Antonio Correia (CMP Cientifica / PHANTOMS-Spain)
Patrick Van Hove (European Commission-Belgium)
Androula G. Nassiopoulou (Institute of Microelectronics, NCSR Demokritos-Greece)
Ramón Compañó (European Commission-Belgium)

Technical Organising Committee:

Nikos Glezos (Institute of Microelectronics, NCSR Demokritos-Greece)
M. Kokonou (Institute of Microelectronics, NCSR Demokritos-Greece)
Cristina Roldán (CMP Científica-Spain)
Fernando Hernández (Fundación PHANTOMS-Spain)

Project Reviews:

Wednesday 4th of February 2004
High-Tree, Sasem, Qudos, Flash, Nice, Sodamos, Mint, Extra, Fracture, Super-ADC, Escher
Friday 6th of February 2004
Nanocold, DNA-nanowires, Nanomagicq, Best, Near, Spinosa, Medics, Molswitch, Nanotera

Previous workshops have been held in Lille (February 1998), Cambridge (July 1998), Marseille (February 1999), Duisburg (July 1999), Pisa (February 2000), Enschede (June 2000), Barcelona (February 2001), Wuerzburg (July 2001), Catania (February 2002), Helsinki (July 2002), Toulouse (February 2003) and Cork (June 2003).

Local Organisation
Dr. Androula G. Nassiopoulou
Institute of Microelectronics, NCSR
Demokritos-Greece
E-mail: A.Nassiopoulou@imel.demokritos.gr

PHANTOMS Organisation
Dr. Antonio Correia
CMP Cientifica / PHANTOMS
E-mail: antonio@phantomsnet.com

Questions regarding **NID Projects & EU**
Dr. Patrick Van Hove
European Commission - DG Information Society
(Future & Emerging Technologies)
Rue de la Loi 200, B-1049 Bruxelles, Belgium
E-mail: Patrick.Van-Hove@cec.eu.int

NANOELECTRONICS CONFERENCES IN EUROPE

(January 2004)

* **Veeco SPM Conference and Users Meeting 2004**
January 12-13, 2004 The Oxford Centre, Oxford, United Kingdom
http://www.veeco-europe.com/uk/spmconf.htm

(February 2004)

* **13th NID Workshop**
February 04-06, 2004 Aghia Paraskevi, Athens, Greece
http://www.phantomsnet.com/nidconference7/index.php

* **Second International Workshop on Multianalyte Biosensing Devices**
February 18-20, 2004 Universitat Rovira i Virgili, Tarragona, Spain
http://www.etseq.urv.es/dinamic/congres/

* **Advances in Molecular Electronics: from molecular materials to single-molecule devices**
February 23-27, 2004 Dresden, Germany
http://www.mpipks-dresden.mpg.de/~admol/

(March 2004)

* **XVIIIth International Winterschool on Electronic Properties of Novel Materials**
March 06-13, 2004 Hotel Sonnalp, Kirchberg / Tirol, Austria
http://www.univie.ac.at/spectroscopy/iwep.htm

* **1st NanoSpain Workshop**
March 10-12, 2004 Palacio Miramar, San Sebastian, Spain
http://www.phantomsnet.com/html/infoC.php?id=375

* **1st International Nanofabrication Symposium**
March 10-12, 2004 Fairways Hotel & Conference Center, Dundalk, Ireland
http://www.nanofabrication.ie/Home.asp

* **NanoScale 2004**
March 25-26, 2004 Braunschweig, Germany
http://www.nanoscale.de/

* **Materials Congress 2004**
March 30 - April 01, 2004 Carlton House Terrace, London, United Kingdom
http://www.iom3.org/congress2004/

NANO-VACANCIES AT PHANTOMS

Post Doctoral Fellow The Computational Modelling Group, NMRC, Ireland has several postdoctoral research and PhD positions open. (http://www.phantomsnet.com/html/infoJ.php?id=355)

Postdoctoral Position at MIC in theory/simulation in an exciting international project on atomic and molecular scale electronic components (Single-Atom And Single-Molecule Electronic Components). Contact: Assoc. Prof. Mads Brandbyge (mbr@mic.dtu.dk) (http://www.phantomsnet.com/html/infoJ.php?id=348)

PostDoctoral Position (Internal Project Manager) at Bioengineering & Bioelectrochemistry Group, Universitat Rovira i Virgili, Spain in Electrochemistry, Nanoelectrochemistry, Nanobiotechnology. Contact: Ioanis Katakis (ikatakis@etseq.urv.es) (http://www.phantomsnet.com/html/infoJ.php?id=358)

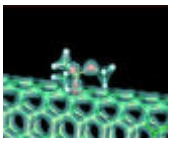
NANONEWS

Weekly updated at http://www.phantomsnet.com

Shown are cobalt nanoparticles that have self-assembled into bracelet-like "nanorings." (Source: Graphic/VCH Publishers)

Purdue's Self-Assembled 'Nanorings' Could Boost Computer Memory Recent nanotechnology research at Purdue University could pave the way toward faster computer memories and higher density magnetic data storage, all with an affordable price tag. (11 December, 2003)
http://www.spacedaily.com/news/nanotech-03zzs.html

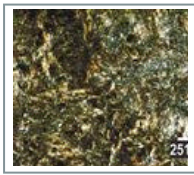
Nanotubes detect nerve gas Naval Research Laboratory researchers have found that carbon nanotubes are sensitive to extremely small concentrations -- less than one part per billion -- of chemical nerve agents. (10 December, 2003)



This graphic shows a dimethyl methylphosphonate (DMMP) molecule connected to a carbon nanotube. The molecule simulates the toxic nerve agent sarin. When the toxin and nanotube are connected, the nanotube's electrical conductivity is reduced. (Source: Naval Research Laboratory)

http://www.trnmag.com/Stories/2003/120303/Nanotubes_detect_nerve_gas_Brief_120303.html

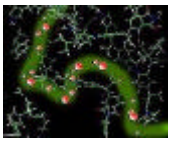
Peptide nanotubes control metal nanocrystals Researchers at the City University of New York, US, have used peptide nanotubes as a template for growing copper nanocrystals. By adjusting the pH of the solution, the scientists were able to control the conformation of the peptide and tailor the diameter of the nanocrystals to between 10 and 30 nm. (09 December, 2003)
http://www.nanotechweb.org/articles/news/2/12/5/1#091203



This image shows a liquid crystalline solution of sulfuric acid and SWNTs. The solution contains roughly 5.5 percent SWNTs by volume; acid dispersions have resulted in over an order of magnitude improvement in concentration over all previously documented methods. (Source: Rice University)

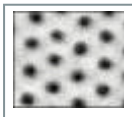
Rice engineers make first pure nanotube fibers Researchers at Rice University have discovered how to create continuous fibers of out of pristine single-walled carbon nanotubes. The process, which is similar to the one used to make Kevlar® on an industrial scale, offers the first real hope of making threads, cables and sheets of pure carbon nanotubes (SWNTs). (09 December, 2003)
http://www.eurekalert.org/pub_releases/2003-12/ru-rem120903.php

Kettering Researchers Discover New Way to Produce Nanotubes Researchers at Kettering University have discovered a different method for producing nanotubes, which is one of the U.S. government's best-funded technology areas. (08 December, 2003)
http://www.spacedaily.com/news/nanotech-03zzq.html



The Kettering team's procedure for creating nanotubes is "actually a simpler way of doing it than had previously been done," said Bahram Roughani, associate professor of Applied Physics. (Source: Kettering University)

Motorola speeds the move to nanocrystal flash Motorola Inc.'s Semiconductor Products Sector has accelerated plans for nanocrystal flash, a form of flash memory that analysts said could extend flash scaling at least to the 45-nanometer node.(08 December, 2003)
http://eetimes.com/semi/news/OEG20031208S0062



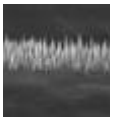
Polymer template: The dark circular holes in the stencil are 20 nanometres in diameter. (Source: IBM)

IBM hails nano chip-making method IBM has trumpeted a nanotech method for making microchip components which it says should enable electronic devices to continue to get smaller and faster. (08 December, 2003)
http://news.bbc.co.uk/2/hi/science/nature/3301025.stm

Tiny 'nanofingers' to support sensors, other applications Engineers here have found an easy way to carve the surface of inexpensive ceramic material into tiny filaments, creating a platform for devices that detect chemicals in the air. They could also be used to clean up toxic chemicals or gather solar energy, or to form fog-free or self-cleaning surfaces. Each filament, or nanofinger, consists of a single crystal of the compound titanium oxide, and measures up to five micrometers long and at most 50 nanometers wide. (08 December, 2003)
http://www.eurekalert.org/pub_releases/2003-12/osu-tt120103.php

Nanodiscs boost polymer lasers Researchers at Ludwig-Maximillians University in Germany believe they have taken a crucial step towards making an electrically-pumped organic polymer laser. By using an array of miniature gold discs as a diffraction grating, the team says its approach could eliminate some of the problems that have held back the development of current-driven devices. (Advanced Materials 15 1726). (05 December, 2003)
http://www.nanotechweb.org/articles/news/2/12/3/1

Scientists grow carbon nanofibres straight onto plastic Researchers from the University of Cambridge, UK, have deposited carbon nanofibres directly onto plastic substrates using plasma-enhanced chemical vapour deposition. The arrays of fibres could have applications as field emitters in displays. (04 December, 2003)
http://www.nanotechweb.org/articles/news/2/12/2/1



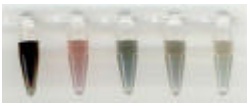
SEM photographs of vertically aligned carbon nanofibres grown directly on flexible plastic foil. (Source: University of Cambridge)

NANONEWS

Weekly updated at http://www.phantomsnet.com

Nano arrays enable terabit-level disks Fundamental materials researchis pushing magnetic media dnsities to new highs. At the Materials Research Society in Boston this week Bruce Terris from the Hitachi San Jose (Calif.) Research Center described a process for creating cobalt-palladium nanoscale islands on silicon dioxide that he believes could carry magnetic media densities into the terabit/square-inch realm. (04 December, 2003)
http://www.eetimes.com/at/news/OEG20031202S0035

DNA sorts out nanotubes Scientists from DuPont, the University of Illinois at Urbana-Champaign and the Massachusetts Institute of Technology, all in the US, have used the self-assembly of DNA to sort carbon nanotubes according to their diameter and electronic properties. The technique could have applications in the processing of inorganic nanomaterials. (03 December, 2003)
http://www.nanotechweb.org/articles/news/2/12/1/1



Fractionated carbon nanotubes. (Source: DuPont, the University of Illinois at Urbana-Champaign and the MIT)

University of Maryland Physicists Show Nanotubes are Best Semiconductors University of Maryland physicists have found that semiconducting carbon nanotubes have the highest mobility of any known material at room temperature. Mobility is a measure of how well a semiconductor conducts electricity. (03 December, 2003)
http://www.ascribe.org/cgi-bin/spew4th.pl?ascribeid=20031203.131754&time=13%2033%20PST&year=2003&public=1

New Production Technique May Let Scientists Fine-Tune Strength and Conductivity of Nanotube-Laced Materials Materials fortified with carbon nanotubes are strongest when the embedded filaments run parallel to each other, but electronic and thermal conductivity are best when the nanotubes are oriented randomly. That the finding from a team of engineers at the University of Pennsylvania who have developed a production technique that permits a finer and more precise dispersion of nanotubes within a material. (02 December, 2003)
http://www.upenn.edu/pennnews/article.php?id=565

Molecular Memories, Once Doubted, Prove Durable and Practical In the ongoing quest to create computing devices that are both incredibly small and incredibly powerful, scientists – envisioning a future beyond the limits of traditional semiconductors – have been working to use molecules for information storage and processing. (01 December, 2003)
http://www.ncsu.edu/news/press_releases/03_12/351.htm

Nanotubes fortify plastic film Researchers from Trinity College in Ireland and Rensselaer Polytechnic Institute have developed an inexpensive process for making a nanotube-polymer composite that allows for close control of the density and position of the nanotubes. (26 November, 2003)
http://www.trnmag.com/Stories/2003/111903/Nanotubes_fortify_plastic_film_Brief_111903.html

DNA self-assembles nanotube transistor Researchers at the Technion-Israel Institute of Technology have used the self-assembly of DNA molecules to build electronic devices from carbon nanotubes. The DNA acts as a scaffold for positioning a single-walled carbon nanotube at the heart of a field-effect transistor, as well as a template for the metallic wires connecting the device (K Keren et al. 2003 Science 302 1380). (24 November, 2003)
http://physicsweb.org/article/news/7/11/13

NEWS

Weekly updated at http://www.phantomsnet.com

Ramon Marimon tells CORDIS News of his role in evaluating the new FP6 instruments As agreed by the Council of Ministers during negotiations on the Sixth Framework Programme (FP6), a mid-term evaluation is to be carried out on the effectiveness of the programme's new instruments - Networks of Excellence and Integrated Projects. The high level expert panel charged with carrying out the evaluation is to be chaired by Ramon Marimon, Spanish Secretary of State for Science and Technology from 2000 until 2002, and a renowned economics researcher at Pompeu Fabra University in Barcelona, which he himself founded. (07 November, 2003)
http://dbs.cordis.lu/fep-cgi/srchidadb?CALLER=FP6_NEWS&ACTION=D&SESSION=&RCN=EN_RCN_ID:21173

Final report of the consultation meeting organised in Brussels on 25 September 2003 A consultation meeting was organised in Brussels on 25 September 2003, as a step towards the definition of the FET proactive initiative to be launched as part of IST Call 3 in 2004.The final report of the workshop identifies a number of promising directions for future research following the successful work of the NID initiative in FP5. (22 October, 2003)
http://www.cordis.lu/ist/fet/nid.htm

EDITORIAL INFORMATION

December 2003, Issue 14.

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Phantoms Newsletter contains information about the European network on nanoelectronics, including scientific review articles, Phantoms members highlights and vacancies, nanoelectronic conferences and nanonews.
Letters to the editor and articles are welcome for publication.

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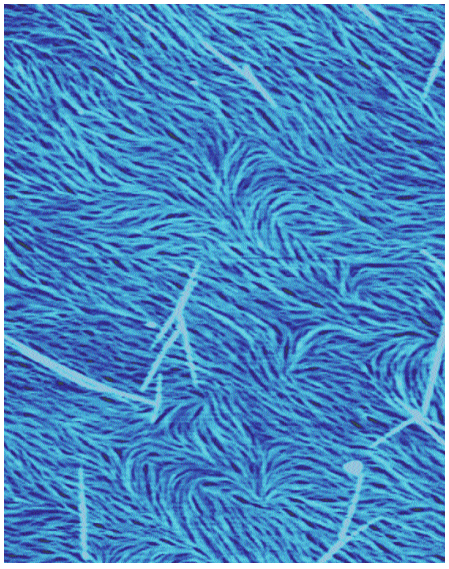

Cover picture:
TM-AFM image of thin deposits of conjugated oligomer-based system: poly(para phenylene ethynylene-poly(di-methylsiloxane). The scan size is 4.0 micrometers. The rigid segments are packed together by pi-stacking in order to form micrometer long semi-conducting nanoribbons. Their width is about few nanometers.
Courtesy of Ph. Leclère and R. Lazzaroni, Laboratory for Chemistry of Novel Materials, University of Mons-Hainaut/Materia Nova (Belgium) [in collaboration with A.C. Grimsdale and K. Müllen, Max-Planck-Institute für Polymerforshung, Mainz (Germany)].